

1/396

Figure 1A-1

	<u>Atom</u>	<u>Type</u>	<u>Resid</u>	<u>#</u>	<u>X</u>	<u>Y</u>	<u>Z</u>	<u>Occ</u>	<u>B</u>
ATOM	1	CB	SER A	19	94.076	71.208	44.896	1.00	0.00
ATOM	2	OG	SER A	19	92.871	71.591	45.534	1.00	0.00
ATOM	3	C	SER A	19	94.111	68.905	45.899	1.00	0.00
ATOM	4	O	SER A	19	94.565	67.868	45.413	1.00	0.00
ATOM	5	N	SER A	19	96.209	69.971	45.139	1.00	0.00
ATOM	6	CA	SER A	19	94.875	70.223	45.758	1.00	0.00
ATOM	7	N	THR A	20	92.957	68.950	46.565	1.00	0.00
ATOM	8	CA	THR A	20	92.134	67.755	46.776	1.00	0.00
ATOM	9	CB	THR A	20	91.314	67.856	48.092	1.00	0.00
ATOM	10	OG1	THR A	20	92.205	67.978	49.207	1.00	0.00
ATOM	11	CG2	THR A	20	90.450	66.615	48.289	1.00	0.00
ATOM	12	C	THR A	20	91.160	67.507	45.627	1.00	0.00
ATOM	13	O	THR A	20	90.572	68.447	45.084	1.00	0.00
ATOM	14	N	ILE A	21	90.994	66.235	45.268	1.00	0.00
ATOM	15	CA	ILE A	21	90.081	65.831	44.198	1.00	0.00
ATOM	16	CB	ILE A	21	90.237	64.325	43.858	1.00	0.00
ATOM	17	CG2	ILE A	21	91.635	64.057	43.324	1.00	0.00
ATOM	18	CG1	ILE A	21	89.942	63.460	45.093	1.00	0.00
ATOM	19	CD1	ILE A	21	90.936	63.600	46.244	1.00	0.00
ATOM	20	C	ILE A	21	88.630	66.096	44.607	1.00	0.00
ATOM	21	O	ILE A	21	87.714	65.381	44.209	1.00	0.00
ATOM	22	N	GLU A	22	88.448	67.134	45.416	1.00	0.00
ATOM	23	CA	GLU A	22	87.148	67.551	45.920	1.00	0.00
ATOM	24	CB	GLU A	22	87.090	67.363	47.440	1.00	0.00
ATOM	25	CG	GLU A	22	85.952	68.105	48.130	1.00	0.00
ATOM	26	CD	GLU A	22	84.637	67.368	48.035	1.00	0.00
ATOM	27	OE1	GLU A	22	84.317	66.881	46.931	1.00	0.00
ATOM	28	OE2	GLU A	22	83.923	67.280	49.060	1.00	0.00
ATOM	29	C	GLU A	22	87.004	69.027	45.593	1.00	0.00
ATOM	30	O	GLU A	22	86.023	69.451	44.984	1.00	0.00
ATOM	31	N	GLU A	23	88.000	69.806	46.003	1.00	0.00
ATOM	32	CA	GLU A	23	87.988	71.239	45.762	1.00	0.00
ATOM	33	CB	GLU A	23	88.992	71.955	46.673	1.00	0.00
ATOM	34	CG	GLU A	23	88.960	73.477	46.538	1.00	0.00
ATOM	35	CD	GLU A	23	87.634	74.086	46.984	1.00	0.00
ATOM	36	OE1	GLU A	23	87.273	75.167	46.469	1.00	0.00
ATOM	37	OE2	GLU A	23	86.959	73.494	47.856	1.00	0.00
ATOM	38	C	GLU A	23	88.315	71.527	44.308	1.00	0.00
ATOM	39	O	GLU A	23	88.020	72.607	43.802	1.00	0.00
ATOM	40	N	GLN A	24	88.941	70.571	43.635	1.00	0.00
ATOM	41	CA	GLN A	24	89.252	70.774	42.229	1.00	0.00
ATOM	42	CB	GLN A	24	90.527	70.014	41.830	1.00	0.00
ATOM	43	CG	GLN A	24	90.488	68.508	42.000	1.00	0.00
ATOM	44	CD	GLN A	24	91.859	67.873	41.805	1.00	0.00
ATOM	45	OE1	GLN A	24	92.514	68.074	40.777	1.00	0.00
ATOM	46	NE2	GLN A	24	92.299	67.102	42.795	1.00	0.00
ATOM	47	C	GLN A	24	88.028	70.313	41.428	1.00	0.00
ATOM	48	O	GLN A	24	87.741	70.833	40.352	1.00	0.00
ATOM	49	N	ALA A	25	87.297	69.350	41.983	1.00	0.00
ATOM	50	CA	ALA A	25	86.083	68.857	41.353	1.00	0.00
ATOM	51	CB	ALA A	25	85.558	67.626	42.082	1.00	0.00
ATOM	52	C	ALA A	25	85.102	70.007	41.498	1.00	0.00

Figure 1A-2

ATOM	53	O	ALA	A	25	84.249	70.234	40.635	1.00	0.00
ATOM	54	N	LYS	A	26	85.232	70.739	42.599	1.00	0.00
ATOM	55	CA	LYS	A	26	84.361	71.875	42.833	1.00	0.00
ATOM	56	CB	LYS	A	26	84.533	72.418	44.253	1.00	0.00
ATOM	57	CG	LYS	A	26	83.840	71.613	45.340	1.00	0.00
ATOM	58	CD	LYS	A	26	83.882	72.371	46.658	1.00	0.00
ATOM	59	CE	LYS	A	26	82.970	71.756	47.697	1.00	0.00
ATOM	60	NZ	LYS	A	26	82.816	72.649	48.876	1.00	0.00
ATOM	61	C	LYS	A	26	84.640	72.984	41.832	1.00	0.00
ATOM	62	O	LYS	A	26	83.719	73.686	41.411	1.00	0.00
ATOM	63	N	THR	A	27	85.902	73.154	41.449	1.00	0.00
ATOM	64	CA	THR	A	27	86.228	74.208	40.498	1.00	0.00
ATOM	65	CB	THR	A	27	87.718	74.641	40.578	1.00	0.00
ATOM	66	OG1	THR	A	27	88.560	73.562	40.171	1.00	0.00
ATOM	67	CG2	THR	A	27	88.076	75.053	42.005	1.00	0.00
ATOM	68	C	THR	A	27	85.893	73.745	39.089	1.00	0.00
ATOM	69	O	THR	A	27	85.542	74.556	38.233	1.00	0.00
ATOM	70	N	PHE	A	28	85.993	72.441	38.855	1.00	0.00
ATOM	71	CA	PHE	A	28	85.651	71.880	37.557	1.00	0.00
ATOM	72	CB	PHE	A	28	85.897	70.373	37.549	1.00	0.00
ATOM	73	CG	PHE	A	28	85.161	69.643	36.455	1.00	0.00
ATOM	74	CD1	PHE	A	28	83.907	69.089	36.689	1.00	0.00
ATOM	75	CD2	PHE	A	28	85.719	69.516	35.187	1.00	0.00
ATOM	76	CE1	PHE	A	28	83.225	68.421	35.686	1.00	0.00
ATOM	77	CE2	PHE	A	28	85.038	68.846	34.171	1.00	0.00
ATOM	78	CZ	PHE	A	28	83.791	68.299	34.423	1.00	0.00
ATOM	79	C	PHE	A	28	84.171	72.165	37.298	1.00	0.00
ATOM	80	O	PHE	A	28	83.798	72.685	36.243	1.00	0.00
ATOM	81	N	LEU	A	29	83.344	71.837	38.285	1.00	0.00
ATOM	82	CA	LEU	A	29	81.907	72.048	38.221	1.00	0.00
ATOM	83	CB	LEU	A	29	81.240	71.472	39.473	1.00	0.00
ATOM	84	CG	LEU	A	29	80.455	70.159	39.384	1.00	0.00
ATOM	85	CD1	LEU	A	29	80.829	69.368	38.144	1.00	0.00
ATOM	86	CD2	LEU	A	29	80.713	69.356	40.649	1.00	0.00
ATOM	87	C	LEU	A	29	81.547	73.520	38.076	1.00	0.00
ATOM	88	O	LEU	A	29	80.617	73.869	37.347	1.00	0.00
ATOM	89	N	ASP	A	30	82.271	74.385	38.775	1.00	0.00
ATOM	90	CA	ASP	A	30	82.009	75.816	38.685	1.00	0.00
ATOM	91	CB	ASP	A	30	82.928	76.591	39.654	1.00	0.00
ATOM	92	CG	ASP	A	30	82.598	78.093	39.725	1.00	0.00
ATOM	93	OD1	ASP	A	30	81.407	78.464	39.821	1.00	0.00
ATOM	94	OD2	ASP	A	30	83.538	78.912	39.702	1.00	0.00
ATOM	95	C	ASP	A	30	82.231	76.272	37.233	1.00	0.00
ATOM	96	O	ASP	A	30	81.443	77.049	36.697	1.00	0.00
ATOM	97	N	LYS	A	31	83.292	75.785	36.597	1.00	0.00
ATOM	98	CA	LYS	A	31	83.572	76.156	35.211	1.00	0.00
ATOM	99	CB	LYS	A	31	84.928	75.593	34.766	1.00	0.00
ATOM	100	CG	LYS	A	31	86.122	76.173	35.526	1.00	0.00
ATOM	101	CD	LYS	A	31	87.450	75.664	34.969	1.00	0.00
ATOM	102	CE	LYS	A	31	88.626	76.120	35.835	1.00	0.00
ATOM	103	NZ	LYS	A	31	89.955	75.761	35.246	1.00	0.00
ATOM	104	C	LYS	A	31	82.452	75.652	34.279	1.00	0.00
ATOM	105	O	LYS	A	31	82.002	76.376	33.382	1.00	0.00
ATOM	106	N	PHE	A	32	82.013	74.414	34.512	1.00	0.00
ATOM	107	CA	PHE	A	32	80.941	73.785	33.746	1.00	0.00
ATOM	108	CB	PHE	A	32	80.681	72.373	34.285	1.00	0.00

Figure 1A-3

ATOM	109	CG	PHE	A	32	79.478	71.706	33.685	1.00	0.00
ATOM	110	CD1	PHE	A	32	78.218	71.859	34.262	1.00	0.00
ATOM	111	CD2	PHE	A	32	79.600	70.941	32.523	1.00	0.00
ATOM	112	CE1	PHE	A	32	77.094	71.256	33.683	1.00	0.00
ATOM	113	CE2	PHE	A	32	78.491	70.343	31.952	1.00	0.00
ATOM	114	CZ	PHE	A	32	77.239	70.500	32.529	1.00	0.00
ATOM	115	C	PHE	A	32	79.640	74.583	33.774	1.00	0.00
ATOM	116	O	PHE	A	32	79.073	74.909	32.732	1.00	0.00
ATOM	117	N	ASN	A	33	79.167	74.898	34.972	1.00	0.00
ATOM	118	CA	ASN	A	33	77.930	75.641	35.126	1.00	0.00
ATOM	119	CB	ASN	A	33	77.659	75.890	36.614	1.00	0.00
ATOM	120	CG	ASN	A	33	77.347	74.605	37.368	1.00	0.00
ATOM	121	OD1	ASN	A	33	77.387	74.564	38.593	1.00	0.00
ATOM	122	ND2	ASN	A	33	77.033	73.546	36.631	1.00	0.00
ATOM	123	C	ASN	A	33	77.907	76.947	34.339	1.00	0.00
ATOM	124	O	ASN	A	33	76.909	77.259	33.681	1.00	0.00
ATOM	125	N	HIS	A	34	79.000	77.705	34.389	1.00	0.00
ATOM	126	CA	HIS	A	34	79.058	78.965	33.654	1.00	0.00
ATOM	127	CB	HIS	A	34	80.243	79.809	34.129	1.00	0.00
ATOM	128	CG	HIS	A	34	80.052	80.381	35.499	1.00	0.00
ATOM	129	CD2	HIS	A	34	80.473	79.947	36.711	1.00	0.00
ATOM	130	ND1	HIS	A	34	79.236	81.468	35.744	1.00	0.00
ATOM	131	CE1	HIS	A	34	79.155	81.672	37.048	1.00	0.00
ATOM	132	NE2	HIS	A	34	79.894	80.760	37.657	1.00	0.00
ATOM	133	C	HIS	A	34	79.123	78.695	32.157	1.00	0.00
ATOM	134	O	HIS	A	34	78.407	79.326	31.388	1.00	0.00
ATOM	135	N	GLU	A	35	79.959	77.756	31.729	1.00	0.00
ATOM	136	CA	GLU	A	35	80.012	77.450	30.306	1.00	0.00
ATOM	137	CB	GLU	A	35	81.167	76.486	29.979	1.00	0.00
ATOM	138	CG	GLU	A	35	82.546	77.148	29.913	1.00	0.00
ATOM	139	CD	GLU	A	35	83.608	76.273	29.261	1.00	0.00
ATOM	140	OE1	GLU	A	35	83.793	75.122	29.710	1.00	0.00
ATOM	141	OE2	GLU	A	35	84.268	76.743	28.304	1.00	0.00
ATOM	142	C	GLU	A	35	78.690	76.837	29.836	1.00	0.00
ATOM	143	O	GLU	A	35	78.111	77.297	28.853	1.00	0.00
ATOM	144	N	ALA	A	36	78.210	75.817	30.554	1.00	0.00
ATOM	145	CA	ALA	A	36	76.965	75.117	30.206	1.00	0.00
ATOM	146	CB	ALA	A	36	76.672	73.985	31.211	1.00	0.00
ATOM	147	C	ALA	A	36	75.783	76.047	30.142	1.00	0.00
ATOM	148	O	ALA	A	36	74.994	75.982	29.210	1.00	0.00
ATOM	149	N	GLU	A	37	75.652	76.918	31.134	1.00	0.00
ATOM	150	CA	GLU	A	37	74.524	77.840	31.154	1.00	0.00
ATOM	151	CB	GLU	A	37	74.612	78.759	32.370	1.00	0.00
ATOM	152	CG	GLU	A	37	73.367	79.587	32.631	1.00	0.00
ATOM	153	CD	GLU	A	37	72.711	79.243	33.960	1.00	0.00
ATOM	154	OE1	GLU	A	37	73.401	78.669	34.843	1.00	0.00
ATOM	155	OE2	GLU	A	37	71.511	79.563	34.125	1.00	0.00
ATOM	156	C	GLU	A	37	74.479	78.684	29.882	1.00	0.00
ATOM	157	O	GLU	A	37	73.404	78.959	29.349	1.00	0.00
ATOM	158	N	ASP	A	38	75.648	79.101	29.401	1.00	0.00
ATOM	159	CA	ASP	A	38	75.717	79.921	28.192	1.00	0.00
ATOM	160	CB	ASP	A	38	77.087	80.595	28.081	1.00	0.00
ATOM	161	CG	ASP	A	38	77.252	81.355	26.781	1.00	0.00
ATOM	162	OD1	ASP	A	38	76.408	82.228	26.490	1.00	0.00
ATOM	163	OD2	ASP	A	38	78.227	81.075	26.049	1.00	0.00
ATOM	164	C	ASP	A	38	75.415	79.133	26.913	1.00	0.00

4/396

Figure 1A-4

ATOM	165	O	ASP	A	38	74.651	79.592	26.075	1.00	0.00
ATOM	166	N	LEU	A	39	75.998	77.950	26.765	1.00	0.00
ATOM	167	CA	LEU	A	39	75.742	77.151	25.570	1.00	0.00
ATOM	168	CB	LEU	A	39	76.720	75.979	25.478	1.00	0.00
ATOM	169	CG	LEU	A	39	78.152	76.349	25.108	1.00	0.00
ATOM	170	CD1	LEU	A	39	79.041	75.115	25.168	1.00	0.00
ATOM	171	CD2	LEU	A	39	78.167	76.952	23.704	1.00	0.00
ATOM	172	C	LEU	A	39	74.316	76.617	25.534	1.00	0.00
ATOM	173	O	LEU	A	39	73.726	76.466	24.458	1.00	0.00
ATOM	174	N	PHE	A	40	73.755	76.320	26.701	1.00	0.00
ATOM	175	CA	PHE	A	40	72.398	75.813	26.738	1.00	0.00
ATOM	176	CB	PHE	A	40	72.046	75.295	28.128	1.00	0.00
ATOM	177	CG	PHE	A	40	70.682	74.657	28.207	1.00	0.00
ATOM	178	CD1	PHE	A	40	70.486	73.348	27.768	1.00	0.00
ATOM	179	CD2	PHE	A	40	69.592	75.372	28.705	1.00	0.00
ATOM	180	CE1	PHE	A	40	69.221	72.754	27.821	1.00	0.00
ATOM	181	CE2	PHE	A	40	68.329	74.796	28.765	1.00	0.00
ATOM	182	CZ	PHE	A	40	68.141	73.482	28.321	1.00	0.00
ATOM	183	C	PHE	A	40	71.448	76.938	26.355	1.00	0.00
ATOM	184	O	PHE	A	40	70.425	76.704	25.708	1.00	0.00
ATOM	185	N	TYR	A	41	71.787	78.159	26.758	1.00	0.00
ATOM	186	CA	TYR	A	41	70.952	79.308	26.432	1.00	0.00
ATOM	187	CB	TYR	A	41	71.425	80.554	27.175	1.00	0.00
ATOM	188	CG	TYR	A	41	70.419	81.674	27.128	1.00	0.00
ATOM	189	CD1	TYR	A	41	69.202	81.560	27.786	1.00	0.00
ATOM	190	CE1	TYR	A	41	68.254	82.579	27.737	1.00	0.00
ATOM	191	CD2	TYR	A	41	70.671	82.843	26.411	1.00	0.00
ATOM	192	CE2	TYR	A	41	69.723	83.874	26.354	1.00	0.00
ATOM	193	CZ	TYR	A	41	68.516	83.732	27.021	1.00	0.00
ATOM	194	OH	TYR	A	41	67.560	84.728	26.969	1.00	0.00
ATOM	195	C	TYR	A	41	70.959	79.594	24.927	1.00	0.00
ATOM	196	O	TYR	A	41	69.923	79.927	24.347	1.00	0.00
ATOM	197	N	GLN	A	42	72.128	79.475	24.302	1.00	0.00
ATOM	198	CA	GLN	A	42	72.250	79.714	22.868	1.00	0.00
ATOM	199	CB	GLN	A	42	73.725	79.686	22.447	1.00	0.00
ATOM	200	CG	GLN	A	42	74.552	80.874	22.980	1.00	0.00
ATOM	201	CD	GLN	A	42	76.063	80.741	22.730	1.00	0.00
ATOM	202	OE1	GLN	A	42	76.516	80.571	21.593	1.00	0.00
ATOM	203	NE2	GLN	A	42	76.843	80.828	23.798	1.00	0.00
ATOM	204	C	GLN	A	42	71.463	78.636	22.125	1.00	0.00
ATOM	205	O	GLN	A	42	70.714	78.927	21.189	1.00	0.00
ATOM	206	N	SER	A	43	71.625	77.392	22.561	1.00	0.00
ATOM	207	CA	SER	A	43	70.928	76.269	21.960	1.00	0.00
ATOM	208	CB	SER	A	43	71.415	74.962	22.570	1.00	0.00
ATOM	209	OG	SER	A	43	70.759	73.863	21.975	1.00	0.00
ATOM	210	C	SER	A	43	69.424	76.385	22.156	1.00	0.00
ATOM	211	O	SER	A	43	68.654	76.047	21.250	1.00	0.00
ATOM	212	N	SER	A	44	69.004	76.858	23.331	1.00	0.00
ATOM	213	CA	SER	A	44	67.583	77.025	23.624	1.00	0.00
ATOM	214	CB	SER	A	44	67.369	77.376	25.101	1.00	0.00
ATOM	215	OG	SER	A	44	67.648	76.269	25.936	1.00	0.00
ATOM	216	C	SER	A	44	66.933	78.103	22.757	1.00	0.00
ATOM	217	O	SER	A	44	65.861	77.883	22.180	1.00	0.00
ATOM	218	N	LEU	A	45	67.577	79.269	22.694	1.00	0.00
ATOM	219	CA	LEU	A	45	67.088	80.397	21.898	1.00	0.00
ATOM	220	CB	LEU	A	45	68.042	81.582	21.999	1.00	0.00

Figure 1A-5

ATOM	221	CG	LEU	A	45	67.610	82.737	22.894	1.00	0.00
ATOM	222	CD1	LEU	A	45	68.811	83.627	23.191	1.00	0.00
ATOM	223	CD2	LEU	A	45	66.496	83.520	22.205	1.00	0.00
ATOM	224	C	LEU	A	45	66.950	80.002	20.438	1.00	0.00
ATOM	225	O	LEU	A	45	66.000	80.384	19.770	1.00	0.00
ATOM	226	N	ALA	A	46	67.913	79.239	19.945	1.00	0.00
ATOM	227	CA	ALA	A	46	67.869	78.785	18.569	1.00	0.00
ATOM	228	CB	ALA	A	46	69.116	77.983	18.244	1.00	0.00
ATOM	229	C	ALA	A	46	66.628	77.926	18.357	1.00	0.00
ATOM	230	O	ALA	A	46	65.857	78.170	17.431	1.00	0.00
ATOM	231	N	SER	A	47	66.438	76.919	19.212	1.00	0.00
ATOM	232	CA	SER	A	47	65.284	76.033	19.095	1.00	0.00
ATOM	233	CB	SER	A	47	65.335	74.924	20.146	1.00	0.00
ATOM	234	OG	SER	A	47	66.327	73.967	19.813	1.00	0.00
ATOM	235	C	SER	A	47	63.973	76.783	19.226	1.00	0.00
ATOM	236	O	SER	A	47	62.967	76.401	18.637	1.00	0.00
ATOM	237	N	TRP	A	48	63.983	77.855	20.000	1.00	0.00
ATOM	238	CA	TRP	A	48	62.778	78.635	20.195	1.00	0.00
ATOM	239	CB	TRP	A	48	62.972	79.601	21.361	1.00	0.00
ATOM	240	CG	TRP	A	48	61.871	80.583	21.495	1.00	0.00
ATOM	241	CD2	TRP	A	48	60.668	80.414	22.247	1.00	0.00
ATOM	242	CE2	TRP	A	48	59.891	81.580	22.058	1.00	0.00
ATOM	243	CE3	TRP	A	48	60.168	79.389	23.062	1.00	0.00
ATOM	244	CD1	TRP	A	48	61.785	81.808	20.895	1.00	0.00
ATOM	245	NE1	TRP	A	48	60.597	82.414	21.230	1.00	0.00
ATOM	246	CZ2	TRP	A	48	58.639	81.751	22.654	1.00	0.00
ATOM	247	CZ3	TRP	A	48	58.923	79.555	23.656	1.00	0.00
ATOM	248	CH2	TRP	A	48	58.171	80.730	23.448	1.00	0.00
ATOM	249	C	TRP	A	48	62.415	79.395	18.925	1.00	0.00
ATOM	250	O	TRP	A	48	61.243	79.578	18.622	1.00	0.00
ATOM	251	N	ASN	A	49	63.431	79.839	18.193	1.00	0.00
ATOM	252	CA	ASN	A	49	63.230	80.572	16.950	1.00	0.00
ATOM	253	CB	ASN	A	49	64.567	81.017	16.369	1.00	0.00
ATOM	254	CG	ASN	A	49	65.159	82.184	17.106	1.00	0.00
ATOM	255	OD1	ASN	A	49	66.355	82.452	16.996	1.00	0.00
ATOM	256	ND2	ASN	A	49	64.326	82.904	17.854	1.00	0.00
ATOM	257	C	ASN	A	49	62.546	79.665	15.954	1.00	0.00
ATOM	258	O	ASN	A	49	61.585	80.063	15.305	1.00	0.00
ATOM	259	N	TYR	A	50	63.053	78.440	15.849	1.00	0.00
ATOM	260	CA	TYR	A	50	62.520	77.441	14.931	1.00	0.00
ATOM	261	CB	TYR	A	50	63.460	76.240	14.887	1.00	0.00
ATOM	262	CG	TYR	A	50	62.905	75.051	14.141	1.00	0.00
ATOM	263	CD1	TYR	A	50	62.982	74.972	12.751	1.00	0.00
ATOM	264	CE1	TYR	A	50	62.485	73.865	12.066	1.00	0.00
ATOM	265	CD2	TYR	A	50	62.310	73.996	14.829	1.00	0.00
ATOM	266	CE2	TYR	A	50	61.810	72.889	14.157	1.00	0.00
ATOM	267	CZ	TYR	A	50	61.902	72.828	12.777	1.00	0.00
ATOM	268	OH	TYR	A	50	61.412	71.727	12.117	1.00	0.00
ATOM	269	C	TYR	A	50	61.100	76.953	15.238	1.00	0.00
ATOM	270	O	TYR	A	50	60.336	76.662	14.312	1.00	0.00
ATOM	271	N	ASN	A	51	60.745	76.847	16.519	1.00	0.00
ATOM	272	CA	ASN	A	51	59.407	76.383	16.887	1.00	0.00
ATOM	273	CB	ASN	A	51	59.407	75.703	18.266	1.00	0.00
ATOM	274	CG	ASN	A	51	60.060	74.334	18.243	1.00	0.00
ATOM	275	OD1	ASN	A	51	61.278	74.218	18.127	1.00	0.00
ATOM	276	ND2	ASN	A	51	59.248	73.286	18.343	1.00	0.00

Figure 1A-6

ATOM	277	C	ASN	A	51	58.388	77.510	16.891	1.00	0.00
ATOM	278	O	ASN	A	51	57.193	77.266	17.037	1.00	0.00
ATOM	279	N	THR	A	52	58.859	78.743	16.740	1.00	0.00
ATOM	280	CA	THR	A	52	57.974	79.905	16.716	1.00	0.00
ATOM	281	CB	THR	A	52	58.457	80.991	17.685	1.00	0.00
ATOM	282	OG1	THR	A	52	59.833	81.289	17.414	1.00	0.00
ATOM	283	CG2	THR	A	52	58.297	80.531	19.126	1.00	0.00
ATOM	284	C	THR	A	52	57.913	80.512	15.316	1.00	0.00
ATOM	285	O	THR	A	52	56.993	81.263	14.989	1.00	0.00
ATOM	286	N	ASN	A	53	58.914	80.186	14.505	1.00	0.00
ATOM	287	CA	ASN	A	53	59.014	80.673	13.138	1.00	0.00
ATOM	288	CB	ASN	A	53	59.807	81.977	13.068	1.00	0.00
ATOM	289	CG	ASN	A	53	59.976	82.476	11.637	1.00	0.00
ATOM	290	OD1	ASN	A	53	60.850	83.299	11.347	1.00	0.00
ATOM	291	ND2	ASN	A	53	59.131	81.982	10.736	1.00	0.00
ATOM	292	C	ASN	A	53	59.741	79.636	12.317	1.00	0.00
ATOM	293	O	ASN	A	53	60.932	79.782	12.046	1.00	0.00
ATOM	294	N	ILE	A	54	59.032	78.584	11.928	1.00	0.00
ATOM	295	CA	ILE	A	54	59.643	77.542	11.129	1.00	0.00
ATOM	296	CB	ILE	A	54	58.611	76.473	10.731	1.00	0.00
ATOM	297	CG2	ILE	A	54	59.276	75.391	9.891	1.00	0.00
ATOM	298	CG1	ILE	A	54	58.002	75.859	11.998	1.00	0.00
ATOM	299	CD1	ILE	A	54	57.053	74.686	11.751	1.00	0.00
ATOM	300	C	ILE	A	54	60.250	78.174	9.882	1.00	0.00
ATOM	301	O	ILE	A	54	59.548	78.779	9.068	1.00	0.00
ATOM	302	N	THR	A	55	61.568	78.048	9.763	1.00	0.00
ATOM	303	CA	THR	A	55	62.332	78.586	8.638	1.00	0.00
ATOM	304	CB	THR	A	55	62.987	79.951	9.011	1.00	0.00
ATOM	305	OG1	THR	A	55	61.994	80.988	8.991	1.00	0.00
ATOM	306	CG2	THR	A	55	64.094	80.306	8.047	1.00	0.00
ATOM	307	C	THR	A	55	63.419	77.565	8.299	1.00	0.00
ATOM	308	O	THR	A	55	63.707	76.672	9.100	1.00	0.00
ATOM	309	N	GLU	A	56	64.011	77.677	7.114	1.00	0.00
ATOM	310	CA	GLU	A	56	65.061	76.745	6.715	1.00	0.00
ATOM	311	CB	GLU	A	56	65.238	76.747	5.194	1.00	0.00
ATOM	312	CG	GLU	A	56	66.258	75.725	4.716	1.00	0.00
ATOM	313	CD	GLU	A	56	65.912	74.318	5.167	1.00	0.00
ATOM	314	OE1	GLU	A	56	66.770	73.415	5.018	1.00	0.00
ATOM	315	OE2	GLU	A	56	64.780	74.117	5.666	1.00	0.00
ATOM	316	C	GLU	A	56	66.395	77.078	7.388	1.00	0.00
ATOM	317	O	GLU	A	56	67.187	76.185	7.698	1.00	0.00
ATOM	318	N	GLU	A	57	66.647	78.366	7.601	1.00	0.00
ATOM	319	CA	GLU	A	57	67.878	78.779	8.252	1.00	0.00
ATOM	320	CB	GLU	A	57	68.291	80.192	7.814	1.00	0.00
ATOM	321	CG	GLU	A	57	67.142	81.145	7.534	1.00	0.00
ATOM	322	CD	GLU	A	57	66.600	81.012	6.117	1.00	0.00
ATOM	323	OE1	GLU	A	57	66.106	79.919	5.760	1.00	0.00
ATOM	324	OE2	GLU	A	57	66.671	82.005	5.358	1.00	0.00
ATOM	325	C	GLU	A	57	67.686	78.728	9.764	1.00	0.00
ATOM	326	O	GLU	A	57	68.658	78.633	10.517	1.00	0.00
ATOM	327	N	ASN	A	58	66.428	78.787	10.200	1.00	0.00
ATOM	328	CA	ASN	A	58	66.119	78.725	11.620	1.00	0.00
ATOM	329	CB	ASN	A	58	64.713	79.256	11.899	1.00	0.00
ATOM	330	CG	ASN	A	58	64.712	80.734	12.255	1.00	0.00
ATOM	331	OD1	ASN	A	58	63.673	81.309	12.571	1.00	0.00
ATOM	332	ND2	ASN	A	58	65.883	81.353	12.209	1.00	0.00

7/396

Figure 1A-7

ATOM	333	C	ASN	A	58	66.261	77.297	12.131	1.00	0.00
ATOM	334	O	ASN	A	58	66.477	77.080	13.324	1.00	0.00
ATOM	335	N	VAL	A	59	66.143	76.325	11.229	1.00	0.00
ATOM	336	CA	VAL	A	59	66.308	74.926	11.612	1.00	0.00
ATOM	337	CB	VAL	A	59	65.666	73.948	10.587	1.00	0.00
ATOM	338	CG1	VAL	A	59	66.553	73.802	9.355	1.00	0.00
ATOM	339	CG2	VAL	A	59	65.445	72.592	11.235	1.00	0.00
ATOM	340	C	VAL	A	59	67.816	74.717	11.616	1.00	0.00
ATOM	341	O	VAL	A	59	68.353	73.958	12.418	1.00	0.00
ATOM	342	N	GLN	A	60	68.484	75.423	10.707	1.00	0.00
ATOM	343	CA	GLN	A	60	69.931	75.371	10.556	1.00	0.00
ATOM	344	CB	GLN	A	60	70.359	76.255	9.375	1.00	0.00
ATOM	345	CG	GLN	A	60	71.872	76.382	9.162	1.00	0.00
ATOM	346	CD	GLN	A	60	72.521	75.109	8.632	1.00	0.00
ATOM	347	OE1	GLN	A	60	73.737	75.064	8.415	1.00	0.00
ATOM	348	NE2	GLN	A	60	71.714	74.072	8.420	1.00	0.00
ATOM	349	C	GLN	A	60	70.594	75.857	11.839	1.00	0.00
ATOM	350	O	GLN	A	60	71.338	75.121	12.476	1.00	0.00
ATOM	351	N	ASN	A	61	70.321	77.101	12.211	1.00	0.00
ATOM	352	CA	ASN	A	61	70.894	77.675	13.419	1.00	0.00
ATOM	353	CB	ASN	A	61	70.297	79.059	13.679	1.00	0.00
ATOM	354	CG	ASN	A	61	70.894	80.131	12.782	1.00	0.00
ATOM	355	OD1	ASN	A	61	70.420	81.266	12.758	1.00	0.00
ATOM	356	ND2	ASN	A	61	71.947	79.779	12.049	1.00	0.00
ATOM	357	C	ASN	A	61	70.659	76.783	14.630	1.00	0.00
ATOM	358	O	ASN	A	61	71.555	76.598	15.458	1.00	0.00
ATOM	359	N	MET	A	62	69.453	76.229	14.725	1.00	0.00
ATOM	360	CA	MET	A	62	69.100	75.363	15.842	1.00	0.00
ATOM	361	CB	MET	A	62	67.606	75.020	15.810	1.00	0.00
ATOM	362	CG	MET	A	62	67.209	73.938	16.814	1.00	0.00
ATOM	363	SD	MET	A	62	65.472	73.445	16.763	1.00	0.00
ATOM	364	CE	MET	A	62	65.436	72.532	15.206	1.00	0.00
ATOM	365	C	MET	A	62	69.912	74.076	15.870	1.00	0.00
ATOM	366	O	MET	A	62	70.524	73.748	16.888	1.00	0.00
ATOM	367	N	ASN	A	63	69.923	73.344	14.760	1.00	0.00
ATOM	368	CA	ASN	A	63	70.662	72.088	14.715	1.00	0.00
ATOM	369	CB	ASN	A	63	70.457	71.382	13.366	1.00	0.00
ATOM	370	CG	ASN	A	63	70.972	72.193	12.189	1.00	0.00
ATOM	371	OD1	ASN	A	63	72.164	72.491	12.099	1.00	0.00
ATOM	372	ND2	ASN	A	63	70.072	72.553	11.275	1.00	0.00
ATOM	373	C	ASN	A	63	72.149	72.290	14.993	1.00	0.00
ATOM	374	O	ASN	A	63	72.798	71.422	15.570	1.00	0.00
ATOM	375	N	ASN	A	64	72.687	73.437	14.593	1.00	0.00
ATOM	376	CA	ASN	A	64	74.097	73.727	14.828	1.00	0.00
ATOM	377	CB	ASN	A	64	74.579	74.843	13.892	1.00	0.00
ATOM	378	CG	ASN	A	64	74.553	74.429	12.427	1.00	0.00
ATOM	379	OD1	ASN	A	64	75.074	73.375	12.062	1.00	0.00
ATOM	380	ND2	ASN	A	64	73.951	75.263	11.581	1.00	0.00
ATOM	381	C	ASN	A	64	74.336	74.132	16.287	1.00	0.00
ATOM	382	O	ASN	A	64	75.330	73.739	16.895	1.00	0.00
ATOM	383	N	ALA	A	65	73.426	74.926	16.840	1.00	0.00
ATOM	384	CA	ALA	A	65	73.546	75.359	18.227	1.00	0.00
ATOM	385	CB	ALA	A	65	72.474	76.393	18.556	1.00	0.00
ATOM	386	C	ALA	A	65	73.375	74.127	19.104	1.00	0.00
ATOM	387	O	ALA	A	65	73.974	74.021	20.177	1.00	0.00
ATOM	388	N	GLY	A	66	72.564	73.192	18.622	1.00	0.00

Figure 1A-8

ATOM	389	CA	GLY	A	66	72.320	71.970	19.358	1.00	0.00
ATOM	390	C	GLY	A	66	73.497	71.014	19.347	1.00	0.00
ATOM	391	O	GLY	A	66	73.778	70.371	20.352	1.00	0.00
ATOM	392	N	ASP	A	67	74.186	70.920	18.215	1.00	0.00
ATOM	393	CA	ASP	A	67	75.340	70.033	18.075	1.00	0.00
ATOM	394	CB	ASP	A	67	75.678	69.855	16.592	1.00	0.00
ATOM	395	CG	ASP	A	67	74.702	68.923	15.879	1.00	0.00
ATOM	396	OD1	ASP	A	67	73.471	69.061	16.087	1.00	0.00
ATOM	397	OD2	ASP	A	67	75.172	68.053	15.108	1.00	0.00
ATOM	398	C	ASP	A	67	76.561	70.554	18.829	1.00	0.00
ATOM	399	O	ASP	A	67	77.471	69.793	19.157	1.00	0.00
ATOM	400	N	LYS	A	68	76.576	71.859	19.084	1.00	0.00
ATOM	401	CA	LYS	A	68	77.656	72.502	19.823	1.00	0.00
ATOM	402	CB	LYS	A	68	77.602	74.023	19.608	1.00	0.00
ATOM	403	CG	LYS	A	68	78.747	74.803	20.235	1.00	0.00
ATOM	404	CD	LYS	A	68	79.236	75.922	19.314	1.00	0.00
ATOM	405	CE	LYS	A	68	79.856	75.356	18.022	1.00	0.00
ATOM	406	NZ	LYS	A	68	80.557	76.374	17.167	1.00	0.00
ATOM	407	C	LYS	A	68	77.468	72.159	21.308	1.00	0.00
ATOM	408	O	LYS	A	68	78.439	71.978	22.044	1.00	0.00
ATOM	409	N	TRP	A	69	76.210	72.060	21.730	1.00	0.00
ATOM	410	CA	TRP	A	69	75.878	71.718	23.106	1.00	0.00
ATOM	411	CB	TRP	A	69	74.389	71.978	23.361	1.00	0.00
ATOM	412	CG	TRP	A	69	73.844	71.371	24.635	1.00	0.00
ATOM	413	CD2	TRP	A	69	74.132	71.779	25.981	1.00	0.00
ATOM	414	CE2	TRP	A	69	73.408	70.919	26.841	1.00	0.00
ATOM	415	CE3	TRP	A	69	74.933	72.784	26.544	1.00	0.00
ATOM	416	CD1	TRP	A	69	72.981	70.312	24.732	1.00	0.00
ATOM	417	NE1	TRP	A	69	72.715	70.037	26.051	1.00	0.00
ATOM	418	CZ2	TRP	A	69	73.458	71.036	28.238	1.00	0.00
ATOM	419	CZ3	TRP	A	69	74.983	72.901	27.934	1.00	0.00
ATOM	420	CH2	TRP	A	69	74.248	72.029	28.764	1.00	0.00
ATOM	421	C	TRP	A	69	76.226	70.259	23.397	1.00	0.00
ATOM	422	O	TRP	A	69	76.802	69.947	24.439	1.00	0.00
ATOM	423	N	SER	A	70	75.887	69.370	22.467	1.00	0.00
ATOM	424	CA	SER	A	70	76.170	67.941	22.625	1.00	0.00
ATOM	425	CB	SER	A	70	75.532	67.145	21.491	1.00	0.00
ATOM	426	OG	SER	A	70	74.129	67.328	21.497	1.00	0.00
ATOM	427	C	SER	A	70	77.660	67.660	22.654	1.00	0.00
ATOM	428	O	SER	A	70	78.119	66.796	23.395	1.00	0.00
ATOM	429	N	ALA	A	71	78.406	68.389	21.837	1.00	0.00
ATOM	430	CA	ALA	A	71	79.850	68.236	21.771	1.00	0.00
ATOM	431	CB	ALA	A	71	80.391	69.007	20.578	1.00	0.00
ATOM	432	C	ALA	A	71	80.499	68.737	23.071	1.00	0.00
ATOM	433	O	ALA	A	71	81.512	68.208	23.517	1.00	0.00
ATOM	434	N	PHE	A	72	79.914	69.775	23.660	1.00	0.00
ATOM	435	CA	PHE	A	72	80.413	70.332	24.914	1.00	0.00
ATOM	436	CB	PHE	A	72	79.685	71.653	25.213	1.00	0.00
ATOM	437	CG	PHE	A	72	79.906	72.178	26.604	1.00	0.00
ATOM	438	CD1	PHE	A	72	81.167	72.601	27.017	1.00	0.00
ATOM	439	CD2	PHE	A	72	78.841	72.269	27.500	1.00	0.00
ATOM	440	CE1	PHE	A	72	81.369	73.112	28.300	1.00	0.00
ATOM	441	CE2	PHE	A	72	79.025	72.779	28.790	1.00	0.00
ATOM	442	CZ	PHE	A	72	80.296	73.202	29.190	1.00	0.00
ATOM	443	C	PHE	A	72	80.152	69.310	26.025	1.00	0.00
ATOM	444	O	PHE	A	72	81.037	68.997	26.826	1.00	0.00

9/396

Figure 1A-9

ATOM	445	N	LEU	A	73	78.934	68.773	26.035	1.00	0.00
ATOM	446	CA	LEU	A	73	78.508	67.798	27.032	1.00	0.00
ATOM	447	CB	LEU	A	73	77.036	67.446	26.808	1.00	0.00
ATOM	448	CG	LEU	A	73	76.095	67.442	28.011	1.00	0.00
ATOM	449	CD1	LEU	A	73	76.191	68.759	28.758	1.00	0.00
ATOM	450	CD2	LEU	A	73	74.674	67.222	27.523	1.00	0.00
ATOM	451	C	LEU	A	73	79.338	66.524	27.015	1.00	0.00
ATOM	452	O	LEU	A	73	79.514	65.877	28.047	1.00	0.00
ATOM	453	N	LYS	A	74	79.847	66.170	25.842	1.00	0.00
ATOM	454	CA	LYS	A	74	80.644	64.962	25.688	1.00	0.00
ATOM	455	CB	LYS	A	74	80.638	64.518	24.221	1.00	0.00
ATOM	456	CG	LYS	A	74	81.227	63.138	23.984	1.00	0.00
ATOM	457	CD	LYS	A	74	81.252	62.797	22.503	1.00	0.00
ATOM	458	CE	LYS	A	74	81.627	61.339	22.281	1.00	0.00
ATOM	459	NZ	LYS	A	74	82.912	60.993	22.957	1.00	0.00
ATOM	460	C	LYS	A	74	82.076	65.179	26.159	1.00	0.00
ATOM	461	O	LYS	A	74	82.667	64.312	26.802	1.00	0.00
ATOM	462	N	GLU	A	75	82.643	66.333	25.832	1.00	0.00
ATOM	463	CA	GLU	A	75	83.999	66.613	26.257	1.00	0.00
ATOM	464	CB	GLU	A	75	84.529	67.888	25.591	1.00	0.00
ATOM	465	CG	GLU	A	75	85.961	68.206	25.997	1.00	0.00
ATOM	466	CD	GLU	A	75	86.445	69.556	25.502	1.00	0.00
ATOM	467	OE1	GLU	A	75	87.628	69.888	25.754	1.00	0.00
ATOM	468	OE2	GLU	A	75	85.647	70.284	24.870	1.00	0.00
ATOM	469	C	GLU	A	75	84.000	66.783	27.778	1.00	0.00
ATOM	470	O	GLU	A	75	84.918	66.327	28.466	1.00	0.00
ATOM	471	N	GLN	A	76	82.960	67.434	28.293	1.00	0.00
ATOM	472	CA	GLN	A	76	82.839	67.676	29.721	1.00	0.00
ATOM	473	CB	GLN	A	76	81.713	68.671	29.979	1.00	0.00
ATOM	474	CG	GLN	A	76	82.013	70.066	29.458	1.00	0.00
ATOM	475	CD	GLN	A	76	83.169	70.714	30.197	1.00	0.00
ATOM	476	OE1	GLN	A	76	83.217	70.695	31.427	1.00	0.00
ATOM	477	NE2	GLN	A	76	84.104	71.295	29.451	1.00	0.00
ATOM	478	C	GLN	A	76	82.596	66.392	30.502	1.00	0.00
ATOM	479	O	GLN	A	76	83.021	66.260	31.651	1.00	0.00
ATOM	480	N	SER	A	77	81.903	65.449	29.879	1.00	0.00
ATOM	481	CA	SER	A	77	81.631	64.173	30.516	1.00	0.00
ATOM	482	CB	SER	A	77	80.596	63.393	29.711	1.00	0.00
ATOM	483	OG	SER	A	77	80.375	62.121	30.286	1.00	0.00
ATOM	484	C	SER	A	77	82.923	63.366	30.594	1.00	0.00
ATOM	485	O	SER	A	77	83.293	62.863	31.648	1.00	0.00
ATOM	486	N	THR	A	78	83.610	63.255	29.466	1.00	0.00
ATOM	487	CA	THR	A	78	84.851	62.503	29.403	1.00	0.00
ATOM	488	CB	THR	A	78	85.127	62.041	27.962	1.00	0.00
ATOM	489	OG1	THR	A	78	85.373	63.181	27.128	1.00	0.00
ATOM	490	CG2	THR	A	78	83.919	61.277	27.420	1.00	0.00
ATOM	491	C	THR	A	78	86.031	63.323	29.915	1.00	0.00
ATOM	492	O	THR	A	78	87.179	63.108	29.510	1.00	0.00
ATOM	493	N	LEU	A	79	85.736	64.259	30.810	1.00	0.00
ATOM	494	CA	LEU	A	79	86.746	65.123	31.404	1.00	0.00
ATOM	495	CB	LEU	A	79	86.636	66.534	30.831	1.00	0.00
ATOM	496	CG	LEU	A	79	87.830	67.481	30.969	1.00	0.00
ATOM	497	CD1	LEU	A	79	89.017	66.946	30.184	1.00	0.00
ATOM	498	CD2	LEU	A	79	87.440	68.853	30.454	1.00	0.00
ATOM	499	C	LEU	A	79	86.450	65.151	32.894	1.00	0.00
ATOM	500	O	LEU	A	79	87.281	65.555	33.702	1.00	0.00

10/396

Figure 1A-10

ATOM	501	N	ALA	A	80	85.244	64.716	33.243	1.00	0.00
ATOM	502	CA	ALA	A	80	84.806	64.665	34.628	1.00	0.00
ATOM	503	CB	ALA	A	80	83.302	64.865	34.706	1.00	0.00
ATOM	504	C	ALA	A	80	85.187	63.321	35.234	1.00	0.00
ATOM	505	O	ALA	A	80	85.214	63.170	36.455	1.00	0.00
ATOM	506	N	GLN	A	81	85.475	62.347	34.375	1.00	0.00
ATOM	507	CA	GLN	A	81	85.861	61.014	34.832	1.00	0.00
ATOM	508	CB	GLN	A	81	86.308	60.152	33.651	1.00	0.00
ATOM	509	CG	GLN	A	81	85.302	60.012	32.513	1.00	0.00
ATOM	510	CD	GLN	A	81	84.019	59.331	32.935	1.00	0.00
ATOM	511	OE1	GLN	A	81	84.013	58.500	33.844	1.00	0.00
ATOM	512	NE2	GLN	A	81	82.922	59.668	32.263	1.00	0.00
ATOM	513	C	GLN	A	81	87.026	61.155	35.809	1.00	0.00
ATOM	514	O	GLN	A	81	87.061	60.519	36.863	1.00	0.00
ATOM	515	N	MET	A	82	87.972	62.006	35.432	1.00	0.00
ATOM	516	CA	MET	A	82	89.169	62.287	36.215	1.00	0.00
ATOM	517	CB	MET	A	82	89.748	63.640	35.779	1.00	0.00
ATOM	518	CG	MET	A	82	91.094	63.998	36.397	1.00	0.00
ATOM	519	SD	MET	A	82	91.662	65.665	35.928	1.00	0.00
ATOM	520	CE	MET	A	82	91.659	66.498	37.533	1.00	0.00
ATOM	521	C	MET	A	82	88.967	62.295	37.731	1.00	0.00
ATOM	522	O	MET	A	82	89.854	61.871	38.472	1.00	0.00
ATOM	523	N	TYR	A	83	87.807	62.762	38.189	1.00	0.00
ATOM	524	CA	TYR	A	83	87.535	62.854	39.625	1.00	0.00
ATOM	525	CB	TYR	A	83	86.708	64.112	39.913	1.00	0.00
ATOM	526	CG	TYR	A	83	87.293	65.334	39.250	1.00	0.00
ATOM	527	CD1	TYR	A	83	86.980	65.649	37.925	1.00	0.00
ATOM	528	CE1	TYR	A	83	87.594	66.714	37.271	1.00	0.00
ATOM	529	CD2	TYR	A	83	88.233	66.124	39.907	1.00	0.00
ATOM	530	CE2	TYR	A	83	88.854	67.189	39.262	1.00	0.00
ATOM	531	CZ	TYR	A	83	88.530	67.475	37.946	1.00	0.00
ATOM	532	OH	TYR	A	83	89.157	68.509	37.301	1.00	0.00
ATOM	533	C	TYR	A	83	86.865	61.636	40.249	1.00	0.00
ATOM	534	O	TYR	A	83	85.655	61.445	40.127	1.00	0.00
ATOM	535	N	PRO	A	84	87.656	60.807	40.954	1.00	0.00
ATOM	536	CD	PRO	A	84	89.068	61.074	41.284	1.00	0.00
ATOM	537	CA	PRO	A	84	87.192	59.588	41.623	1.00	0.00
ATOM	538	CB	PRO	A	84	88.343	59.256	42.569	1.00	0.00
ATOM	539	CG	PRO	A	84	89.538	59.734	41.813	1.00	0.00
ATOM	540	C	PRO	A	84	85.881	59.796	42.369	1.00	0.00
ATOM	541	O	PRO	A	84	85.813	60.567	43.327	1.00	0.00
ATOM	542	N	LEU	A	85	84.843	59.106	41.916	1.00	0.00
ATOM	543	CA	LEU	A	85	83.532	59.200	42.535	1.00	0.00
ATOM	544	CB	LEU	A	85	82.550	58.265	41.815	1.00	0.00
ATOM	545	CG	LEU	A	85	82.885	56.767	41.723	1.00	0.00
ATOM	546	CD1	LEU	A	85	81.783	56.051	40.947	1.00	0.00
ATOM	547	CD2	LEU	A	85	84.230	56.556	41.032	1.00	0.00
ATOM	548	C	LEU	A	85	83.594	58.860	44.027	1.00	0.00
ATOM	549	O	LEU	A	85	82.905	59.482	44.838	1.00	0.00
ATOM	550	N	GLN	A	86	84.429	57.887	44.388	1.00	0.00
ATOM	551	CA	GLN	A	86	84.557	57.479	45.785	1.00	0.00
ATOM	552	CB	GLN	A	86	85.249	56.112	45.888	1.00	0.00
ATOM	553	CG	GLN	A	86	85.258	55.540	47.306	1.00	0.00
ATOM	554	CD	GLN	A	86	85.840	54.133	47.390	1.00	0.00
ATOM	555	OE1	GLN	A	86	87.014	53.911	47.088	1.00	0.00
ATOM	556	NE2	GLN	A	86	85.015	53.175	47.808	1.00	0.00

Figure 1A-11

ATOM	557	C	GLN	A	86	85.316	58.509	46.624	1.00	0.00
ATOM	558	O	GLN	A	86	84.989	58.732	47.792	1.00	0.00
ATOM	559	N	GLU	A	87	86.327	59.135	46.031	1.00	0.00
ATOM	560	CA	GLU	A	87	87.109	60.143	46.739	1.00	0.00
ATOM	561	CB	GLU	A	87	88.340	60.538	45.918	1.00	0.00
ATOM	562	CG	GLU	A	87	89.670	59.921	46.356	1.00	0.00
ATOM	563	CD	GLU	A	87	89.711	58.409	46.225	1.00	0.00
ATOM	564	OE1	GLU	A	87	89.257	57.714	47.161	1.00	0.00
ATOM	565	OE2	GLU	A	87	90.193	57.915	45.180	1.00	0.00
ATOM	566	C	GLU	A	87	86.265	61.389	46.995	1.00	0.00
ATOM	567	O	GLU	A	87	86.775	62.396	47.481	1.00	0.00
ATOM	568	N	ILE	A	88	84.976	61.316	46.669	1.00	0.00
ATOM	569	CA	ILE	A	88	84.071	62.451	46.847	1.00	0.00
ATOM	570	CB	ILE	A	88	83.125	62.605	45.633	1.00	0.00
ATOM	571	CG2	ILE	A	88	82.265	63.853	45.800	1.00	0.00
ATOM	572	CG1	ILE	A	88	83.942	62.681	44.337	1.00	0.00
ATOM	573	CD1	ILE	A	88	84.910	63.859	44.262	1.00	0.00
ATOM	574	C	ILE	A	88	83.222	62.364	48.114	1.00	0.00
ATOM	575	O	ILE	A	88	82.637	61.324	48.415	1.00	0.00
ATOM	576	N	GLN	A	89	83.149	63.480	48.835	1.00	0.00
ATOM	577	CA	GLN	A	89	82.398	63.565	50.082	1.00	0.00
ATOM	578	CB	GLN	A	89	83.266	64.239	51.147	1.00	0.00
ATOM	579	CG	GLN	A	89	82.506	64.757	52.357	1.00	0.00
ATOM	580	CD	GLN	A	89	83.368	65.642	53.242	1.00	0.00
ATOM	581	OE1	GLN	A	89	84.364	65.190	53.810	1.00	0.00
ATOM	582	NE2	GLN	A	89	82.992	66.913	53.357	1.00	0.00
ATOM	583	C	GLN	A	89	81.085	64.325	49.942	1.00	0.00
ATOM	584	O	GLN	A	89	80.017	63.796	50.256	1.00	0.00
ATOM	585	N	ASN	A	90	81.176	65.574	49.493	1.00	0.00
ATOM	586	CA	ASN	A	90	80.007	66.434	49.305	1.00	0.00
ATOM	587	CB	ASN	A	90	80.455	67.773	48.718	1.00	0.00
ATOM	588	CG	ASN	A	90	79.384	68.837	48.808	1.00	0.00
ATOM	589	OD1	ASN	A	90	78.247	68.620	48.382	1.00	0.00
ATOM	590	ND2	ASN	A	90	79.758	69.989	49.362	1.00	0.00
ATOM	591	C	ASN	A	90	79.006	65.756	48.361	1.00	0.00
ATOM	592	O	ASN	A	90	79.260	65.633	47.164	1.00	0.00
ATOM	593	N	LEU	A	91	77.873	65.315	48.901	1.00	0.00
ATOM	594	CA	LEU	A	91	76.859	64.633	48.100	1.00	0.00
ATOM	595	CB	LEU	A	91	75.720	64.130	48.997	1.00	0.00
ATOM	596	CG	LEU	A	91	76.074	63.035	50.008	1.00	0.00
ATOM	597	CD1	LEU	A	91	77.070	63.572	51.022	1.00	0.00
ATOM	598	CD2	LEU	A	91	74.816	62.559	50.713	1.00	0.00
ATOM	599	C	LEU	A	91	76.291	65.509	46.984	1.00	0.00
ATOM	600	O	LEU	A	91	75.891	65.009	45.930	1.00	0.00
ATOM	601	N	THR	A	92	76.255	66.815	47.213	1.00	0.00
ATOM	602	CA	THR	A	92	75.742	67.729	46.208	1.00	0.00
ATOM	603	CB	THR	A	92	75.638	69.155	46.755	1.00	0.00
ATOM	604	OG1	THR	A	92	74.813	69.150	47.925	1.00	0.00
ATOM	605	CG2	THR	A	92	75.028	70.086	45.713	1.00	0.00
ATOM	606	C	THR	A	92	76.662	67.737	44.993	1.00	0.00
ATOM	607	O	THR	A	92	76.191	67.826	43.853	1.00	0.00
ATOM	608	N	VAL	A	93	77.971	67.646	45.230	1.00	0.00
ATOM	609	CA	VAL	A	93	78.915	67.644	44.126	1.00	0.00
ATOM	610	CB	VAL	A	93	80.339	68.059	44.561	1.00	0.00
ATOM	611	CG1	VAL	A	93	80.284	69.378	45.312	1.00	0.00
ATOM	612	CG2	VAL	A	93	80.970	66.978	45.394	1.00	0.00

Figure 1A-12

ATOM	613	C	VAL	A	93	78.973	66.265	43.503	1.00	0.00
ATOM	614	O	VAL	A	93	79.331	66.129	42.336	1.00	0.00
ATOM	615	N	LYS	A	94	78.615	65.240	44.273	1.00	0.00
ATOM	616	CA	LYS	A	94	78.623	63.881	43.740	1.00	0.00
ATOM	617	CB	LYS	A	94	78.433	62.830	44.850	1.00	0.00
ATOM	618	CG	LYS	A	94	78.844	61.419	44.402	1.00	0.00
ATOM	619	CD	LYS	A	94	78.465	60.311	45.391	1.00	0.00
ATOM	620	CE	LYS	A	94	76.986	59.920	45.268	1.00	0.00
ATOM	621	NZ	LYS	A	94	76.611	58.721	46.089	1.00	0.00
ATOM	622	C	LYS	A	94	77.483	63.767	42.726	1.00	0.00
ATOM	623	O	LYS	A	94	77.649	63.182	41.660	1.00	0.00
ATOM	624	N	LEU	A	95	76.327	64.334	43.069	1.00	0.00
ATOM	625	CA	LEU	A	95	75.166	64.316	42.180	1.00	0.00
ATOM	626	CB	LEU	A	95	74.021	65.151	42.762	1.00	0.00
ATOM	627	CG	LEU	A	95	73.287	64.566	43.963	1.00	0.00
ATOM	628	CD1	LEU	A	95	72.254	65.573	44.469	1.00	0.00
ATOM	629	CD2	LEU	A	95	72.633	63.248	43.565	1.00	0.00
ATOM	630	C	LEU	A	95	75.543	64.881	40.821	1.00	0.00
ATOM	631	O	LEU	A	95	75.398	64.209	39.801	1.00	0.00
ATOM	632	N	GLN	A	96	76.022	66.122	40.819	1.00	0.00
ATOM	633	CA	GLN	A	96	76.424	66.800	39.590	1.00	0.00
ATOM	634	CB	GLN	A	96	76.995	68.169	39.920	1.00	0.00
ATOM	635	CG	GLN	A	96	75.958	69.204	40.200	1.00	0.00
ATOM	636	CD	GLN	A	96	76.539	70.399	40.910	1.00	0.00
ATOM	637	OE1	GLN	A	96	76.760	70.360	42.116	1.00	0.00
ATOM	638	NE2	GLN	A	96	76.801	71.464	40.167	1.00	0.00
ATOM	639	C	GLN	A	96	77.464	65.996	38.833	1.00	0.00
ATOM	640	O	GLN	A	96	77.341	65.766	37.629	1.00	0.00
ATOM	641	N	LEU	A	97	78.493	65.576	39.556	1.00	0.00
ATOM	642	CA	LEU	A	97	79.573	64.801	38.977	1.00	0.00
ATOM	643	CB	LEU	A	97	80.612	64.514	40.054	1.00	0.00
ATOM	644	CG	LEU	A	97	82.008	64.048	39.653	1.00	0.00
ATOM	645	CD1	LEU	A	97	82.676	65.088	38.750	1.00	0.00
ATOM	646	CD2	LEU	A	97	82.824	63.834	40.923	1.00	0.00
ATOM	647	C	LEU	A	97	78.995	63.506	38.428	1.00	0.00
ATOM	648	O	LEU	A	97	79.357	63.055	37.344	1.00	0.00
ATOM	649	N	GLN	A	98	78.073	62.922	39.181	1.00	0.00
ATOM	650	CA	GLN	A	98	77.433	61.676	38.787	1.00	0.00
ATOM	651	CB	GLN	A	98	76.423	61.254	39.861	1.00	0.00
ATOM	652	CG	GLN	A	98	75.981	59.800	39.788	1.00	0.00
ATOM	653	CD	GLN	A	98	75.189	59.373	41.018	1.00	0.00
ATOM	654	OE1	GLN	A	98	74.090	59.875	41.276	1.00	0.00
ATOM	655	NE2	GLN	A	98	75.750	58.446	41.786	1.00	0.00
ATOM	656	C	GLN	A	98	76.736	61.843	37.435	1.00	0.00
ATOM	657	O	GLN	A	98	76.974	61.076	36.499	1.00	0.00
ATOM	658	N	ALA	A	99	75.881	62.852	37.332	1.00	0.00
ATOM	659	CA	ALA	A	99	75.165	63.101	36.092	1.00	0.00
ATOM	660	CB	ALA	A	99	74.353	64.377	36.215	1.00	0.00
ATOM	661	C	ALA	A	99	76.129	63.199	34.907	1.00	0.00
ATOM	662	O	ALA	A	99	75.911	62.577	33.863	1.00	0.00
ATOM	663	N	LEU	A	100	77.202	63.965	35.086	1.00	0.00
ATOM	664	CA	LEU	A	100	78.197	64.180	34.043	1.00	0.00
ATOM	665	CB	LEU	A	100	79.147	65.310	34.460	1.00	0.00
ATOM	666	CG	LEU	A	100	78.694	66.738	34.147	1.00	0.00
ATOM	667	CD1	LEU	A	100	79.759	67.742	34.565	1.00	0.00
ATOM	668	CD2	LEU	A	100	78.436	66.851	32.657	1.00	0.00

Figure 1A-13

ATOM	669	C	LEU	A	100	79.032	62.995	33.547	1.00	0.00
ATOM	670	O	LEU	A	100	79.164	62.801	32.335	1.00	0.00
ATOM	671	N	GLN	A	101	79.604	62.206	34.455	1.00	0.00
ATOM	672	CA	GLN	A	101	80.446	61.093	34.021	1.00	0.00
ATOM	673	CB	GLN	A	101	81.545	60.813	35.051	1.00	0.00
ATOM	674	CG	GLN	A	101	81.082	60.642	36.471	1.00	0.00
ATOM	675	CD	GLN	A	101	82.244	60.368	37.403	1.00	0.00
ATOM	676	OE1	GLN	A	101	82.914	59.337	37.289	1.00	0.00
ATOM	677	NE2	GLN	A	101	82.502	61.295	38.322	1.00	0.00
ATOM	678	C	GLN	A	101	79.721	59.805	33.671	1.00	0.00
ATOM	679	O	GLN	A	101	80.217	58.705	33.920	1.00	0.00
ATOM	680	N	GLN	A	102	78.552	59.959	33.064	1.00	0.00
ATOM	681	CA	GLN	A	102	77.734	58.835	32.639	1.00	0.00
ATOM	682	CB	GLN	A	102	76.265	59.177	32.872	1.00	0.00
ATOM	683	CG	GLN	A	102	75.289	58.057	32.633	1.00	0.00
ATOM	684	CD	GLN	A	102	73.854	58.520	32.820	1.00	0.00
ATOM	685	OE1	GLN	A	102	73.481	59.006	33.893	1.00	0.00
ATOM	686	NE2	GLN	A	102	73.041	58.378	31.775	1.00	0.00
ATOM	687	C	GLN	A	102	78.020	58.656	31.147	1.00	0.00
ATOM	688	O	GLN	A	102	77.588	59.472	30.331	1.00	0.00
ATOM	689	N	ASN	A	103	78.754	57.600	30.794	1.00	0.00
ATOM	690	CA	ASN	A	103	79.115	57.357	29.397	1.00	0.00
ATOM	691	CB	ASN	A	103	80.177	56.258	29.294	1.00	0.00
ATOM	692	CG	ASN	A	103	81.506	56.668	29.900	1.00	0.00
ATOM	693	OD1	ASN	A	103	81.914	57.827	29.804	1.00	0.00
ATOM	694	ND2	ASN	A	103	82.192	55.704	30.506	1.00	0.00
ATOM	695	C	ASN	A	103	77.955	57.008	28.473	1.00	0.00
ATOM	696	O	ASN	A	103	77.796	57.616	27.415	1.00	0.00
ATOM	697	N	GLY	A	104	77.155	56.020	28.859	1.00	0.00
ATOM	698	CA	GLY	A	104	76.029	55.630	28.031	1.00	0.00
ATOM	699	C	GLY	A	104	76.447	54.849	26.799	1.00	0.00
ATOM	700	O	GLY	A	104	77.160	53.855	26.904	1.00	0.00
ATOM	701	N	SER	A	105	76.004	55.305	25.630	1.00	0.00
ATOM	702	CA	SER	A	105	76.316	54.641	24.369	1.00	0.00
ATOM	703	CB	SER	A	105	75.393	55.159	23.264	1.00	0.00
ATOM	704	OG	SER	A	105	74.037	54.897	23.586	1.00	0.00
ATOM	705	C	SER	A	105	77.767	54.813	23.943	1.00	0.00
ATOM	706	O	SER	A	105	78.318	53.952	23.246	1.00	0.00
ATOM	707	N	SER	A	106	78.379	55.923	24.357	1.00	0.00
ATOM	708	CA	SER	A	106	79.776	56.204	24.020	1.00	0.00
ATOM	709	CB	SER	A	106	80.210	57.561	24.590	1.00	0.00
ATOM	710	OG	SER	A	106	80.410	57.495	25.997	1.00	0.00
ATOM	711	C	SER	A	106	80.682	55.109	24.577	1.00	0.00
ATOM	712	O	SER	A	106	81.875	55.072	24.285	1.00	0.00
ATOM	713	N	VAL	A	107	80.104	54.219	25.380	1.00	0.00
ATOM	714	CA	VAL	A	107	80.846	53.118	25.978	1.00	0.00
ATOM	715	CB	VAL	A	107	80.179	52.639	27.287	1.00	0.00
ATOM	716	CG1	VAL	A	107	79.058	51.657	26.978	1.00	0.00
ATOM	717	CG2	VAL	A	107	81.208	52.016	28.195	1.00	0.00
ATOM	718	C	VAL	A	107	80.907	51.957	24.992	1.00	0.00
ATOM	719	O	VAL	A	107	81.498	50.921	25.276	1.00	0.00
ATOM	720	N	LEU	A	108	80.285	52.141	23.833	1.00	0.00
ATOM	721	CA	LEU	A	108	80.269	51.120	22.789	1.00	0.00
ATOM	722	CB	LEU	A	108	78.895	51.066	22.104	1.00	0.00
ATOM	723	CG	LEU	A	108	77.702	50.466	22.856	1.00	0.00
ATOM	724	CD1	LEU	A	108	76.418	50.777	22.093	1.00	0.00

Figure 1A-14

ATOM	725	CD2	LEU	A	108	77.892	48.960	23.018	1.00	0.00
ATOM	726	C	LEU	A	108	81.326	51.414	21.733	1.00	0.00
ATOM	727	O	LEU	A	108	81.745	52.558	21.564	1.00	0.00
ATOM	728	N	SER	A	109	81.749	50.372	21.021	1.00	0.00
ATOM	729	CA	SER	A	109	82.735	50.528	19.964	1.00	0.00
ATOM	730	CB	SER	A	109	83.090	49.173	19.369	1.00	0.00
ATOM	731	OG	SER	A	109	82.024	48.693	18.578	1.00	0.00
ATOM	732	C	SER	A	109	82.085	51.401	18.895	1.00	0.00
ATOM	733	O	SER	A	109	80.864	51.514	18.846	1.00	0.00
ATOM	734	N	GLU	A	110	82.894	52.007	18.035	1.00	0.00
ATOM	735	CA	GLU	A	110	82.374	52.880	16.989	1.00	0.00
ATOM	736	CB	GLU	A	110	83.529	53.432	16.151	1.00	0.00
ATOM	737	CG	GLU	A	110	83.111	54.428	15.076	1.00	0.00
ATOM	738	CD	GLU	A	110	82.226	55.549	15.613	1.00	0.00
ATOM	739	OE1	GLU	A	110	81.031	55.292	15.893	1.00	0.00
ATOM	740	OE2	GLU	A	110	82.728	56.686	15.762	1.00	0.00
ATOM	741	C	GLU	A	110	81.349	52.200	16.080	1.00	0.00
ATOM	742	O	GLU	A	110	80.313	52.785	15.765	1.00	0.00
ATOM	743	N	ASP	A	111	81.635	50.970	15.664	1.00	0.00
ATOM	744	CA	ASP	A	111	80.728	50.234	14.789	1.00	0.00
ATOM	745	CB	ASP	A	111	81.418	48.990	14.217	1.00	0.00
ATOM	746	CG	ASP	A	111	82.569	49.336	13.276	1.00	0.00
ATOM	747	OD1	ASP	A	111	82.454	50.335	12.526	1.00	0.00
ATOM	748	OD2	ASP	A	111	83.582	48.600	13.275	1.00	0.00
ATOM	749	C	ASP	A	111	79.430	49.820	15.482	1.00	0.00
ATOM	750	O	ASP	A	111	78.412	49.620	14.821	1.00	0.00
ATOM	751	N	LYS	A	112	79.470	49.682	16.806	1.00	0.00
ATOM	752	CA	LYS	A	112	78.284	49.303	17.566	1.00	0.00
ATOM	753	CB	LYS	A	112	78.676	48.790	18.960	1.00	0.00
ATOM	754	CG	LYS	A	112	79.401	47.430	18.984	1.00	0.00
ATOM	755	CD	LYS	A	112	78.506	46.289	18.528	1.00	0.00
ATOM	756	CE	LYS	A	112	79.191	44.931	18.682	1.00	0.00
ATOM	757	NZ	LYS	A	112	79.504	44.587	20.098	1.00	0.00
ATOM	758	C	LYS	A	112	77.359	50.517	17.705	1.00	0.00
ATOM	759	O	LYS	A	112	76.163	50.437	17.435	1.00	0.00
ATOM	760	N	SER	A	113	77.936	51.637	18.128	1.00	0.00
ATOM	761	CA	SER	A	113	77.199	52.877	18.309	1.00	0.00
ATOM	762	CB	SER	A	113	78.147	53.984	18.770	1.00	0.00
ATOM	763	OG	SER	A	113	78.646	53.706	20.061	1.00	0.00
ATOM	764	C	SER	A	113	76.528	53.302	17.014	1.00	0.00
ATOM	765	O	SER	A	113	75.400	53.792	17.018	1.00	0.00
ATOM	766	N	LYS	A	114	77.238	53.117	15.911	1.00	0.00
ATOM	767	CA	LYS	A	114	76.731	53.480	14.603	1.00	0.00
ATOM	768	CB	LYS	A	114	77.831	53.276	13.546	1.00	0.00
ATOM	769	CG	LYS	A	114	77.716	54.160	12.290	1.00	0.00
ATOM	770	CD	LYS	A	114	76.471	53.831	11.468	1.00	0.00
ATOM	771	CE	LYS	A	114	76.321	54.756	10.266	1.00	0.00
ATOM	772	NZ	LYS	A	114	76.084	56.163	10.679	1.00	0.00
ATOM	773	C	LYS	A	114	75.515	52.610	14.288	1.00	0.00
ATOM	774	O	LYS	A	114	74.468	53.111	13.870	1.00	0.00
ATOM	775	N	ARG	A	115	75.651	51.306	14.502	1.00	0.00
ATOM	776	CA	ARG	A	115	74.554	50.385	14.216	1.00	0.00
ATOM	777	CB	ARG	A	115	75.018	48.934	14.387	1.00	0.00
ATOM	778	CG	ARG	A	115	73.950	47.889	14.135	1.00	0.00
ATOM	779	CD	ARG	A	115	73.382	47.981	12.726	1.00	0.00
ATOM	780	NE	ARG	A	115	72.331	46.987	12.512	1.00	0.00

Figure 1A-15

ATOM	781	CZ	ARG	A	115	71.484	46.991	11.489	1.00	0.00
ATOM	782	NH1	ARG	A	115	70.565	46.040	11.392	1.00	0.00
ATOM	783	NH2	ARG	A	115	71.546	47.944	10.567	1.00	0.00
ATOM	784	C	ARG	A	115	73.356	50.679	15.112	1.00	0.00
ATOM	785	O	ARG	A	115	72.222	50.734	14.633	1.00	0.00
ATOM	786	N	LEU	A	116	73.606	50.893	16.402	1.00	0.00
ATOM	787	CA	LEU	A	116	72.523	51.191	17.332	1.00	0.00
ATOM	788	CB	LEU	A	116	73.046	51.395	18.761	1.00	0.00
ATOM	789	CG	LEU	A	116	72.005	51.924	19.765	1.00	0.00
ATOM	790	CD1	LEU	A	116	70.831	50.957	19.825	1.00	0.00
ATOM	791	CD2	LEU	A	116	72.618	52.095	21.158	1.00	0.00
ATOM	792	C	LEU	A	116	71.783	52.445	16.881	1.00	0.00
ATOM	793	O	LEU	A	116	70.553	52.468	16.876	1.00	0.00
ATOM	794	N	ASN	A	117	72.519	53.484	16.494	1.00	0.00
ATOM	795	CA	ASN	A	117	71.873	54.714	16.053	1.00	0.00
ATOM	796	CB	ASN	A	117	72.910	55.829	15.840	1.00	0.00
ATOM	797	CG	ASN	A	117	73.383	56.437	17.155	1.00	0.00
ATOM	798	OD1	ASN	A	117	72.674	56.375	18.173	1.00	0.00
ATOM	799	ND2	ASN	A	117	74.573	57.039	17.143	1.00	0.00
ATOM	800	C	ASN	A	117	71.056	54.483	14.786	1.00	0.00
ATOM	801	O	ASN	A	117	69.972	55.041	14.626	1.00	0.00
ATOM	802	N	THR	A	118	71.579	53.653	13.894	1.00	0.00
ATOM	803	CA	THR	A	118	70.883	53.315	12.668	1.00	0.00
ATOM	804	CB	THR	A	118	71.764	52.409	11.789	1.00	0.00
ATOM	805	OG1	THR	A	118	72.946	53.127	11.424	1.00	0.00
ATOM	806	CG2	THR	A	118	71.040	51.996	10.531	1.00	0.00
ATOM	807	C	THR	A	118	69.579	52.606	13.051	1.00	0.00
ATOM	808	O	THR	A	118	68.505	52.990	12.606	1.00	0.00
ATOM	809	N	ILE	A	119	69.664	51.597	13.907	1.00	0.00
ATOM	810	CA	ILE	A	119	68.460	50.897	14.330	1.00	0.00
ATOM	811	CB	ILE	A	119	68.770	49.753	15.315	1.00	0.00
ATOM	812	CG2	ILE	A	119	67.479	49.183	15.875	1.00	0.00
ATOM	813	CG1	ILE	A	119	69.519	48.638	14.586	1.00	0.00
ATOM	814	CD1	ILE	A	119	69.930	47.502	15.493	1.00	0.00
ATOM	815	C	ILE	A	119	67.447	51.827	14.979	1.00	0.00
ATOM	816	O	ILE	A	119	66.255	51.719	14.727	1.00	0.00
ATOM	817	N	LEU	A	120	67.898	52.737	15.829	1.00	0.00
ATOM	818	CA	LEU	A	120	66.944	53.649	16.456	1.00	0.00
ATOM	819	CB	LEU	A	120	67.640	54.533	17.503	1.00	0.00
ATOM	820	CG	LEU	A	120	68.113	53.821	18.783	1.00	0.00
ATOM	821	CD1	LEU	A	120	69.029	54.741	19.616	1.00	0.00
ATOM	822	CD2	LEU	A	120	66.893	53.394	19.604	1.00	0.00
ATOM	823	C	LEU	A	120	66.265	54.517	15.384	1.00	0.00
ATOM	824	O	LEU	A	120	65.035	54.637	15.356	1.00	0.00
ATOM	825	N	ASN	A	121	67.057	55.099	14.486	1.00	0.00
ATOM	826	CA	ASN	A	121	66.486	55.953	13.450	1.00	0.00
ATOM	827	CB	ASN	A	121	67.594	56.624	12.634	1.00	0.00
ATOM	828	CG	ASN	A	121	68.345	57.672	13.444	1.00	0.00
ATOM	829	OD1	ASN	A	121	67.735	58.466	14.168	1.00	0.00
ATOM	830	ND2	ASN	A	121	69.670	57.682	13.327	1.00	0.00
ATOM	831	C	ASN	A	121	65.537	55.198	12.544	1.00	0.00
ATOM	832	O	ASN	A	121	64.499	55.729	12.141	1.00	0.00
ATOM	833	N	THR	A	122	65.883	53.954	12.243	1.00	0.00
ATOM	834	CA	THR	A	122	65.054	53.124	11.389	1.00	0.00
ATOM	835	CB	THR	A	122	65.778	51.814	11.020	1.00	0.00
ATOM	836	OG1	THR	A	122	67.079	52.128	10.514	1.00	0.00

Figure 1A-16

ATOM	837	CG2	THR	A	122	64.998	51.043	9.943	1.00	0.00
ATOM	838	C	THR	A	122	63.724	52.798	12.067	1.00	0.00
ATOM	839	O	THR	A	122	62.675	53.002	11.466	1.00	0.00
ATOM	840	N	MET	A	123	63.756	52.308	13.311	1.00	0.00
ATOM	841	CA	MET	A	123	62.513	51.971	14.003	1.00	0.00
ATOM	842	CB	MET	A	123	62.766	51.450	15.435	1.00	0.00
ATOM	843	CG	MET	A	123	63.473	50.097	15.553	1.00	0.00
ATOM	844	SD	MET	A	123	63.322	49.349	17.218	1.00	0.00
ATOM	845	CE	MET	A	123	64.398	50.469	18.217	1.00	0.00
ATOM	846	C	MET	A	123	61.657	53.219	14.095	1.00	0.00
ATOM	847	O	MET	A	123	60.435	53.181	13.936	1.00	0.00
ATOM	848	N	SER	A	124	62.308	54.338	14.363	1.00	0.00
ATOM	849	CA	SER	A	124	61.580	55.579	14.500	1.00	0.00
ATOM	850	CB	SER	A	124	62.522	56.690	14.939	1.00	0.00
ATOM	851	OG	SER	A	124	61.779	57.854	15.208	1.00	0.00
ATOM	852	C	SER	A	124	60.859	56.007	13.224	1.00	0.00
ATOM	853	O	SER	A	124	59.721	56.480	13.270	1.00	0.00
ATOM	854	N	THR	A	125	61.521	55.847	12.090	1.00	0.00
ATOM	855	CA	THR	A	125	60.920	56.269	10.843	1.00	0.00
ATOM	856	CB	THR	A	125	61.975	56.456	9.725	1.00	0.00
ATOM	857	OG1	THR	A	125	62.571	55.197	9.416	1.00	0.00
ATOM	858	CG2	THR	A	125	63.057	57.418	10.172	1.00	0.00
ATOM	859	C	THR	A	125	59.827	55.331	10.368	1.00	0.00
ATOM	860	O	THR	A	125	58.792	55.809	9.924	1.00	0.00
ATOM	861	N	ILE	A	126	60.016	54.012	10.473	1.00	0.00
ATOM	862	CA	ILE	A	126	58.949	53.130	10.013	1.00	0.00
ATOM	863	CB	ILE	A	126	59.329	51.620	10.062	1.00	0.00
ATOM	864	CG2	ILE	A	126	60.781	51.409	9.693	1.00	0.00
ATOM	865	CG1	ILE	A	126	59.042	51.052	11.433	1.00	0.00
ATOM	866	CD1	ILE	A	126	57.704	50.365	11.494	1.00	0.00
ATOM	867	C	ILE	A	126	57.707	53.368	10.867	1.00	0.00
ATOM	868	O	ILE	A	126	56.591	53.175	10.391	1.00	0.00
ATOM	869	N	TYR	A	127	57.893	53.801	12.118	1.00	0.00
ATOM	870	CA	TYR	A	127	56.761	54.086	13.007	1.00	0.00
ATOM	871	CB	TYR	A	127	57.240	54.306	14.459	1.00	0.00
ATOM	872	CG	TYR	A	127	56.113	54.598	15.440	1.00	0.00
ATOM	873	CD1	TYR	A	127	55.676	55.904	15.701	1.00	0.00
ATOM	874	CE1	TYR	A	127	54.603	56.137	16.554	1.00	0.00
ATOM	875	CD2	TYR	A	127	55.443	53.551	16.064	1.00	0.00
ATOM	876	CE2	TYR	A	127	54.378	53.775	16.902	1.00	0.00
ATOM	877	CZ	TYR	A	127	53.963	55.044	17.146	1.00	0.00
ATOM	878	OH	TYR	A	127	52.901	55.180	18.009	1.00	0.00
ATOM	879	C	TYR	A	127	55.990	55.337	12.584	1.00	0.00
ATOM	880	O	TYR	A	127	54.756	55.379	12.621	1.00	0.00
ATOM	881	N	SER	A	128	56.717	56.375	12.198	1.00	0.00
ATOM	882	CA	SER	A	128	56.047	57.616	11.838	1.00	0.00
ATOM	883	CB	SER	A	128	56.917	58.818	12.196	1.00	0.00
ATOM	884	OG	SER	A	128	58.089	58.814	11.410	1.00	0.00
ATOM	885	C	SER	A	128	55.706	57.691	10.370	1.00	0.00
ATOM	886	O	SER	A	128	54.981	58.572	9.967	1.00	0.00
ATOM	887	N	THR	A	129	56.191	56.741	9.586	1.00	0.00
ATOM	888	CA	THR	A	129	55.951	56.782	8.162	1.00	0.00
ATOM	889	CB	THR	A	129	57.283	57.089	7.443	1.00	0.00
ATOM	890	OG1	THR	A	129	57.005	57.666	6.168	1.00	0.00
ATOM	891	CG2	THR	A	129	58.119	55.837	7.272	1.00	0.00
ATOM	892	C	THR	A	129	55.291	55.525	7.597	1.00	0.00

Figure 1A-17

ATOM	893	O	THR	A	129	54.911	55.479	6.429	1.00	0.00
ATOM	894	N	GLY	A	130	55.137	54.512	8.438	1.00	0.00
ATOM	895	CA	GLY	A	130	54.511	53.286	7.994	1.00	0.00
ATOM	896	C	GLY	A	130	53.039	53.513	7.736	1.00	0.00
ATOM	897	O	GLY	A	130	52.408	54.381	8.350	1.00	0.00
ATOM	898	N	LYS	A	131	52.478	52.741	6.818	1.00	0.00
ATOM	899	CA	LYS	A	131	51.066	52.887	6.511	1.00	0.00
ATOM	900	CB	LYS	A	131	50.868	53.930	5.400	1.00	0.00
ATOM	901	CG	LYS	A	131	51.673	53.685	4.146	1.00	0.00
ATOM	902	CD	LYS	A	131	51.453	54.825	3.147	1.00	0.00
ATOM	903	CE	LYS	A	131	51.719	56.192	3.790	1.00	0.00
ATOM	904	NZ	LYS	A	131	51.384	57.347	2.903	1.00	0.00
ATOM	905	C	LYS	A	131	50.409	51.579	6.117	1.00	0.00
ATOM	906	O	LYS	A	131	51.071	50.623	5.726	1.00	0.00
ATOM	907	N	VAL	A	132	49.095	51.525	6.239	1.00	0.00
ATOM	908	CA	VAL	A	132	48.392	50.315	5.854	1.00	0.00
ATOM	909	CB	VAL	A	132	47.622	49.685	7.049	1.00	0.00
ATOM	910	CG1	VAL	A	132	48.592	49.293	8.130	1.00	0.00
ATOM	911	CG2	VAL	A	132	46.609	50.648	7.592	1.00	0.00
ATOM	912	C	VAL	A	132	47.424	50.739	4.767	1.00	0.00
ATOM	913	O	VAL	A	132	47.019	51.901	4.713	1.00	0.00
ATOM	914	N	CYS	A	133	47.055	49.818	3.891	1.00	0.00
ATOM	915	CA	CYS	A	133	46.136	50.188	2.827	1.00	0.00
ATOM	916	C	CYS	A	133	44.875	49.336	2.852	1.00	0.00
ATOM	917	O	CYS	A	133	44.895	48.189	3.298	1.00	0.00
ATOM	918	CB	CYS	A	133	46.820	50.069	1.464	1.00	0.00
ATOM	919	SG	CYS	A	133	48.427	50.922	1.285	1.00	0.00
ATOM	920	N	ASN	A	134	43.779	49.923	2.383	1.00	0.00
ATOM	921	CA	ASN	A	134	42.495	49.254	2.319	1.00	0.00
ATOM	922	CB	ASN	A	134	41.456	50.206	1.745	1.00	0.00
ATOM	923	CG	ASN	A	134	40.078	49.586	1.681	1.00	0.00
ATOM	924	OD1	ASN	A	134	39.938	48.388	1.460	1.00	0.00
ATOM	925	ND2	ASN	A	134	39.049	50.407	1.859	1.00	0.00
ATOM	926	C	ASN	A	134	42.579	48.003	1.438	1.00	0.00
ATOM	927	O	ASN	A	134	43.078	48.055	0.312	1.00	0.00
ATOM	928	N	PRO	A	135	42.084	46.859	1.940	1.00	0.00
ATOM	929	CD	PRO	A	135	41.464	46.618	3.254	1.00	0.00
ATOM	930	CA	PRO	A	135	42.133	45.624	1.155	1.00	0.00
ATOM	931	CB	PRO	A	135	41.523	44.587	2.098	1.00	0.00
ATOM	932	CG	PRO	A	135	41.772	45.163	3.474	1.00	0.00
ATOM	933	C	PRO	A	135	41.349	45.740	-0.156	1.00	0.00
ATOM	934	O	PRO	A	135	41.722	45.142	-1.162	1.00	0.00
ATOM	935	N	ASP	A	136	40.269	46.516	-0.140	1.00	0.00
ATOM	936	CA	ASP	A	136	39.448	46.688	-1.328	1.00	0.00
ATOM	937	CB	ASP	A	136	37.973	46.898	-0.940	1.00	0.00
ATOM	938	CG	ASP	A	136	37.564	48.367	-0.919	1.00	0.00
ATOM	939	OD1	ASP	A	136	37.620	48.991	0.167	1.00	0.00
ATOM	940	OD2	ASP	A	136	37.186	48.897	-1.995	1.00	0.00
ATOM	941	C	ASP	A	136	39.935	47.837	-2.212	1.00	0.00
ATOM	942	O	ASP	A	136	39.386	48.075	-3.293	1.00	0.00
ATOM	943	N	ASN	A	137	40.967	48.545	-1.757	1.00	0.00
ATOM	944	CA	ASN	A	137	41.528	49.651	-2.528	1.00	0.00
ATOM	945	CB	ASN	A	137	40.674	50.907	-2.360	1.00	0.00
ATOM	946	CG	ASN	A	137	41.180	52.069	-3.190	1.00	0.00
ATOM	947	OD1	ASN	A	137	40.592	53.150	-3.183	1.00	0.00
ATOM	948	ND2	ASN	A	137	42.274	51.856	-3.909	1.00	0.00

Figure 1A-18

ATOM	949	C	ASN	A	137	42.961	49.930	-2.093	1.00	0.00
ATOM	950	O	ASN	A	137	43.203	50.747	-1.211	1.00	0.00
ATOM	951	N	PRO	A	138	43.931	49.250	-2.730	1.00	0.00
ATOM	952	CD	PRO	A	138	43.664	48.237	-3.767	1.00	0.00
ATOM	953	CA	PRO	A	138	45.370	49.354	-2.477	1.00	0.00
ATOM	954	CB	PRO	A	138	45.968	48.444	-3.542	1.00	0.00
ATOM	955	CG	PRO	A	138	44.912	47.393	-3.719	1.00	0.00
ATOM	956	C	PRO	A	138	45.934	50.767	-2.563	1.00	0.00
ATOM	957	O	PRO	A	138	47.076	51.004	-2.177	1.00	0.00
ATOM	958	N	GLN	A	139	45.139	51.701	-3.073	1.00	0.00
ATOM	959	CA	GLN	A	139	45.597	53.077	-3.212	1.00	0.00
ATOM	960	CB	GLN	A	139	45.143	53.648	-4.565	1.00	0.00
ATOM	961	CG	GLN	A	139	45.975	53.159	-5.759	1.00	0.00
ATOM	962	CD	GLN	A	139	45.796	51.680	-6.046	1.00	0.00
ATOM	963	OE1	GLN	A	139	46.769	50.923	-6.105	1.00	0.00
ATOM	964	NE2	GLN	A	139	44.547	51.257	-6.223	1.00	0.00
ATOM	965	C	GLN	A	139	45.126	53.969	-2.052	1.00	0.00
ATOM	966	O	GLN	A	139	45.564	55.109	-1.908	1.00	0.00
ATOM	967	N	GLU	A	140	44.232	53.442	-1.227	1.00	0.00
ATOM	968	CA	GLU	A	140	43.765	54.194	-0.080	1.00	0.00
ATOM	969	CB	GLU	A	140	42.296	53.890	0.209	1.00	0.00
ATOM	970	CG	GLU	A	140	41.651	54.910	1.125	1.00	0.00
ATOM	971	CD	GLU	A	140	40.426	54.371	1.829	1.00	0.00
ATOM	972	OE1	GLU	A	140	39.520	53.852	1.142	1.00	0.00
ATOM	973	OE2	GLU	A	140	40.370	54.474	3.074	1.00	0.00
ATOM	974	C	GLU	A	140	44.639	53.692	1.060	1.00	0.00
ATOM	975	O	GLU	A	140	44.465	52.577	1.543	1.00	0.00
ATOM	976	N	CYS	A	141	45.605	54.500	1.465	1.00	0.00
ATOM	977	CA	CYS	A	141	46.507	54.098	2.528	1.00	0.00
ATOM	978	C	CYS	A	141	46.506	55.135	3.650	1.00	0.00
ATOM	979	O	CYS	A	141	46.466	56.340	3.402	1.00	0.00
ATOM	980	CB	CYS	A	141	47.915	53.911	1.959	1.00	0.00
ATOM	981	SG	CYS	A	141	48.021	52.773	0.527	1.00	0.00
ATOM	982	N	LEU	A	142	46.537	54.655	4.885	1.00	0.00
ATOM	983	CA	LEU	A	142	46.510	55.522	6.054	1.00	0.00
ATOM	984	CB	LEU	A	142	45.300	55.184	6.927	1.00	0.00
ATOM	985	CG	LEU	A	142	43.892	55.206	6.322	1.00	0.00
ATOM	986	CD1	LEU	A	142	42.944	54.469	7.257	1.00	0.00
ATOM	987	CD2	LEU	A	142	43.425	56.649	6.099	1.00	0.00
ATOM	988	C	LEU	A	142	47.759	55.396	6.919	1.00	0.00
ATOM	989	O	LEU	A	142	48.337	54.316	7.047	1.00	0.00
ATOM	990	N	LEU	A	143	48.164	56.514	7.505	1.00	0.00
ATOM	991	CA	LEU	A	143	49.295	56.547	8.412	1.00	0.00
ATOM	992	CB	LEU	A	143	49.992	57.918	8.397	1.00	0.00
ATOM	993	CG	LEU	A	143	50.886	58.332	7.221	1.00	0.00
ATOM	994	CD1	LEU	A	143	50.148	58.130	5.911	1.00	0.00
ATOM	995	CD2	LEU	A	143	51.277	59.796	7.368	1.00	0.00
ATOM	996	C	LEU	A	143	48.643	56.359	9.770	1.00	0.00
ATOM	997	O	LEU	A	143	47.420	56.454	9.893	1.00	0.00
ATOM	998	N	LEU	A	144	49.454	56.094	10.789	1.00	0.00
ATOM	999	CA	LEU	A	144	48.926	55.942	12.140	1.00	0.00
ATOM	1000	CB	LEU	A	144	50.064	55.683	13.134	1.00	0.00
ATOM	1001	CG	LEU	A	144	49.572	55.694	14.574	1.00	0.00
ATOM	1002	CD1	LEU	A	144	48.501	54.606	14.718	1.00	0.00
ATOM	1003	CD2	LEU	A	144	50.733	55.464	15.545	1.00	0.00
ATOM	1004	C	LEU	A	144	48.243	57.255	12.512	1.00	0.00

Figure 1A-19

ATOM	1005	O	LEU	A	144	47.129	57.274	13.033	1.00	0.00
ATOM	1006	N	GLU	A	145	48.937	58.351	12.243	1.00	0.00
ATOM	1007	CA	GLU	A	145	48.435	59.683	12.563	1.00	0.00
ATOM	1008	CB	GLU	A	145	49.353	60.347	13.591	1.00	0.00
ATOM	1009	CG	GLU	A	145	49.001	61.795	13.913	1.00	0.00
ATOM	1010	CD	GLU	A	145	47.625	61.967	14.549	1.00	0.00
ATOM	1011	OE1	GLU	A	145	47.100	61.019	15.169	1.00	0.00
ATOM	1012	OE2	GLU	A	145	47.068	63.081	14.448	1.00	0.00
ATOM	1013	C	GLU	A	145	48.341	60.594	11.342	1.00	0.00
ATOM	1014	O	GLU	A	145	49.357	60.938	10.739	1.00	0.00
ATOM	1015	N	PRO	A	146	47.120	60.980	10.952	1.00	0.00
ATOM	1016	CD	PRO	A	146	46.878	61.999	9.906	1.00	0.00
ATOM	1017	CA	PRO	A	146	45.866	60.598	11.600	1.00	0.00
ATOM	1018	CB	PRO	A	146	45.005	61.834	11.396	1.00	0.00
ATOM	1019	CG	PRO	A	146	45.363	62.209	9.965	1.00	0.00
ATOM	1020	C	PRO	A	146	45.387	59.421	10.768	1.00	0.00
ATOM	1021	O	PRO	A	146	46.162	58.856	10.002	1.00	0.00
ATOM	1022	N	GLY	A	147	44.135	59.031	10.889	1.00	0.00
ATOM	1023	CA	GLY	A	147	43.698	57.936	10.041	1.00	0.00
ATOM	1024	C	GLY	A	147	43.423	56.705	10.850	1.00	0.00
ATOM	1025	O	GLY	A	147	42.278	56.412	11.179	1.00	0.00
ATOM	1026	N	LEU	A	148	44.484	55.980	11.175	1.00	0.00
ATOM	1027	CA	LEU	A	148	44.345	54.789	11.979	1.00	0.00
ATOM	1028	CB	LEU	A	148	45.678	54.043	12.006	1.00	0.00
ATOM	1029	CG	LEU	A	148	45.720	52.716	11.237	1.00	0.00
ATOM	1030	CD1	LEU	A	148	44.832	52.738	10.011	1.00	0.00
ATOM	1031	CD2	LEU	A	148	47.157	52.416	10.862	1.00	0.00
ATOM	1032	C	LEU	A	148	43.911	55.245	13.374	1.00	0.00
ATOM	1033	O	LEU	A	148	43.033	54.637	13.996	1.00	0.00
ATOM	1034	N	ASN	A	149	44.508	56.329	13.855	1.00	0.00
ATOM	1035	CA	ASN	A	149	44.154	56.868	15.162	1.00	0.00
ATOM	1036	CB	ASN	A	149	45.059	58.052	15.527	1.00	0.00
ATOM	1037	CG	ASN	A	149	46.415	57.626	16.093	1.00	0.00
ATOM	1038	OD1	ASN	A	149	47.338	58.432	16.139	1.00	0.00
ATOM	1039	ND2	ASN	A	149	46.533	56.369	16.535	1.00	0.00
ATOM	1040	C	ASN	A	149	42.720	57.367	15.124	1.00	0.00
ATOM	1041	O	ASN	A	149	41.951	57.162	16.076	1.00	0.00
ATOM	1042	N	GLU	A	150	42.354	58.030	14.026	1.00	0.00
ATOM	1043	CA	GLU	A	150	41.002	58.579	13.910	1.00	0.00
ATOM	1044	CB	GLU	A	150	40.840	59.367	12.610	1.00	0.00
ATOM	1045	CG	GLU	A	150	39.524	60.144	12.526	1.00	0.00
ATOM	1046	CD	GLU	A	150	38.324	59.257	12.182	1.00	0.00
ATOM	1047	OE1	GLU	A	150	37.177	59.634	12.525	1.00	0.00
ATOM	1048	OE2	GLU	A	150	38.529	58.192	11.552	1.00	0.00
ATOM	1049	C	GLU	A	150	39.984	57.463	13.983	1.00	0.00
ATOM	1050	O	GLU	A	150	38.935	57.602	14.620	1.00	0.00
ATOM	1051	N	ILE	A	151	40.306	56.348	13.336	1.00	0.00
ATOM	1052	CA	ILE	A	151	39.437	55.180	13.338	1.00	0.00
ATOM	1053	CB	ILE	A	151	39.974	54.068	12.409	1.00	0.00
ATOM	1054	CG2	ILE	A	151	39.220	52.772	12.670	1.00	0.00
ATOM	1055	CG1	ILE	A	151	39.856	54.482	10.942	1.00	0.00
ATOM	1056	CD1	ILE	A	151	40.489	53.472	10.006	1.00	0.00
ATOM	1057	C	ILE	A	151	39.351	54.564	14.726	1.00	0.00
ATOM	1058	O	ILE	A	151	38.264	54.355	15.252	1.00	0.00
ATOM	1059	N	MET	A	152	40.508	54.249	15.307	1.00	0.00
ATOM	1060	CA	MET	A	152	40.542	53.605	16.613	1.00	0.00

Figure 1A-20

ATOM	1061	CB	MET	A	152	41.988	53.263	16.999	1.00	0.00
ATOM	1062	CG	MET	A	152	42.665	52.281	16.033	1.00	0.00
ATOM	1063	SD	MET	A	152	41.625	50.802	15.743	1.00	0.00
ATOM	1064	CE	MET	A	152	41.803	49.959	17.393	1.00	0.00
ATOM	1065	C	MET	A	152	39.870	54.408	17.710	1.00	0.00
ATOM	1066	O	MET	A	152	39.435	53.852	18.728	1.00	0.00
ATOM	1067	N	ALA	A	153	39.747	55.711	17.495	1.00	0.00
ATOM	1068	CA	ALA	A	153	39.119	56.560	18.492	1.00	0.00
ATOM	1069	CB	ALA	A	153	39.858	57.890	18.579	1.00	0.00
ATOM	1070	C	ALA	A	153	37.639	56.819	18.235	1.00	0.00
ATOM	1071	O	ALA	A	153	36.870	57.036	19.186	1.00	0.00
ATOM	1072	N	ASN	A	154	37.221	56.770	16.971	1.00	0.00
ATOM	1073	CA	ASN	A	154	35.828	57.093	16.663	1.00	0.00
ATOM	1074	CB	ASN	A	154	35.792	58.336	15.766	1.00	0.00
ATOM	1075	CG	ASN	A	154	36.543	59.519	16.374	1.00	0.00
ATOM	1076	OD1	ASN	A	154	37.592	59.931	15.877	1.00	0.00
ATOM	1077	ND2	ASN	A	154	36.013	60.058	17.461	1.00	0.00
ATOM	1078	C	ASN	A	154	34.918	56.020	16.063	1.00	0.00
ATOM	1079	O	ASN	A	154	33.696	56.128	16.170	1.00	0.00
ATOM	1080	N	SER	A	155	35.495	54.987	15.460	1.00	0.00
ATOM	1081	CA	SER	A	155	34.706	53.939	14.829	1.00	0.00
ATOM	1082	CB	SER	A	155	35.595	53.097	13.912	1.00	0.00
ATOM	1083	OG	SER	A	155	34.914	51.931	13.478	1.00	0.00
ATOM	1084	C	SER	A	155	33.973	53.021	15.791	1.00	0.00
ATOM	1085	O	SER	A	155	34.474	52.723	16.876	1.00	0.00
ATOM	1086	N	LEU	A	156	32.784	52.568	15.377	1.00	0.00
ATOM	1087	CA	LEU	A	156	31.975	51.656	16.185	1.00	0.00
ATOM	1088	CB	LEU	A	156	30.618	52.274	16.542	1.00	0.00
ATOM	1089	CG	LEU	A	156	30.583	53.265	17.712	1.00	0.00
ATOM	1090	CD1	LEU	A	156	31.601	54.354	17.487	1.00	0.00
ATOM	1091	CD2	LEU	A	156	29.198	53.883	17.831	1.00	0.00
ATOM	1092	C	LEU	A	156	31.747	50.357	15.439	1.00	0.00
ATOM	1093	O	LEU	A	156	30.889	49.561	15.819	1.00	0.00
ATOM	1094	N	ASP	A	157	32.508	50.145	14.371	1.00	0.00
ATOM	1095	CA	ASP	A	157	32.380	48.923	13.588	1.00	0.00
ATOM	1096	CB	ASP	A	157	32.511	49.217	12.101	1.00	0.00
ATOM	1097	CG	ASP	A	157	32.532	47.950	11.273	1.00	0.00
ATOM	1098	OD1	ASP	A	157	31.456	47.496	10.841	1.00	0.00
ATOM	1099	OD2	ASP	A	157	33.623	47.383	11.079	1.00	0.00
ATOM	1100	C	ASP	A	157	33.458	47.913	13.984	1.00	0.00
ATOM	1101	O	ASP	A	157	34.642	48.141	13.777	1.00	0.00
ATOM	1102	N	TYR	A	158	33.038	46.791	14.539	1.00	0.00
ATOM	1103	CA	TYR	A	158	33.960	45.757	14.972	1.00	0.00
ATOM	1104	CB	TYR	A	158	33.168	44.509	15.376	1.00	0.00
ATOM	1105	CG	TYR	A	158	33.988	43.415	16.024	1.00	0.00
ATOM	1106	CD1	TYR	A	158	34.091	43.324	17.411	1.00	0.00
ATOM	1107	CE1	TYR	A	158	34.831	42.300	18.016	1.00	0.00
ATOM	1108	CD2	TYR	A	158	34.652	42.459	15.253	1.00	0.00
ATOM	1109	CE2	TYR	A	158	35.396	41.442	15.849	1.00	0.00
ATOM	1110	CZ	TYR	A	158	35.477	41.369	17.229	1.00	0.00
ATOM	1111	OH	TYR	A	158	36.205	40.364	17.828	1.00	0.00
ATOM	1112	C	TYR	A	158	34.999	45.391	13.910	1.00	0.00
ATOM	1113	O	TYR	A	158	36.198	45.341	14.198	1.00	0.00
ATOM	1114	N	ASN	A	159	34.551	45.143	12.682	1.00	0.00
ATOM	1115	CA	ASN	A	159	35.481	44.750	11.625	1.00	0.00
ATOM	1116	CB	ASN	A	159	34.716	44.220	10.414	1.00	0.00

21/396

Figure 1A-21

ATOM	1117	CG	ASN	A	159	33.812	43.063	10.772	1.00	0.00
ATOM	1118	OD1	ASN	A	159	34.215	42.142	11.492	1.00	0.00
ATOM	1119	ND2	ASN	A	159	32.580	43.096	10.265	1.00	0.00
ATOM	1120	C	ASN	A	159	36.462	45.815	11.172	1.00	0.00
ATOM	1121	O	ASN	A	159	37.616	45.513	10.897	1.00	0.00
ATOM	1122	N	GLU	A	160	36.008	47.058	11.081	1.00	0.00
ATOM	1123	CA	GLU	A	160	36.890	48.139	10.663	1.00	0.00
ATOM	1124	CB	GLU	A	160	36.079	49.422	10.469	1.00	0.00
ATOM	1125	CG	GLU	A	160	36.883	50.552	9.869	1.00	0.00
ATOM	1126	CD	GLU	A	160	36.158	51.876	9.944	1.00	0.00
ATOM	1127	OE1	GLU	A	160	36.603	52.840	9.280	1.00	0.00
ATOM	1128	OE2	GLU	A	160	35.142	51.957	10.670	1.00	0.00
ATOM	1129	C	GLU	A	160	37.988	48.349	11.733	1.00	0.00
ATOM	1130	O	GLU	A	160	39.171	48.485	11.410	1.00	0.00
ATOM	1131	N	ARG	A	161	37.589	48.376	13.002	1.00	0.00
ATOM	1132	CA	ARG	A	161	38.546	48.545	14.092	1.00	0.00
ATOM	1133	CB	ARG	A	161	37.831	48.597	15.452	1.00	0.00
ATOM	1134	CG	ARG	A	161	36.942	49.804	15.665	1.00	0.00
ATOM	1135	CD	ARG	A	161	36.368	49.811	17.081	1.00	0.00
ATOM	1136	NE	ARG	A	161	37.437	50.038	18.041	1.00	0.00
ATOM	1137	CZ	ARG	A	161	37.839	51.239	18.429	1.00	0.00
ATOM	1138	NH1	ARG	A	161	37.244	52.330	17.960	1.00	0.00
ATOM	1139	NH2	ARG	A	161	38.883	51.351	19.230	1.00	0.00
ATOM	1140	C	ARG	A	161	39.535	47.379	14.081	1.00	0.00
ATOM	1141	O	ARG	A	161	40.727	47.561	14.321	1.00	0.00
ATOM	1142	N	LEU	A	162	39.036	46.181	13.793	1.00	0.00
ATOM	1143	CA	LEU	A	162	39.891	45.006	13.766	1.00	0.00
ATOM	1144	CB	LEU	A	162	39.057	43.724	13.625	1.00	0.00
ATOM	1145	CG	LEU	A	162	39.870	42.443	13.400	1.00	0.00
ATOM	1146	CD1	LEU	A	162	40.800	42.247	14.583	1.00	0.00
ATOM	1147	CD2	LEU	A	162	38.951	41.227	13.240	1.00	0.00
ATOM	1148	C	LEU	A	162	40.859	45.120	12.606	1.00	0.00
ATOM	1149	O	LEU	A	162	42.051	44.816	12.736	1.00	0.00
ATOM	1150	N	TRP	A	163	40.352	45.546	11.455	1.00	0.00
ATOM	1151	CA	TRP	A	163	41.215	45.696	10.300	1.00	0.00
ATOM	1152	CB	TRP	A	163	40.444	46.265	9.107	1.00	0.00
ATOM	1153	CG	TRP	A	163	41.409	46.737	8.063	1.00	0.00
ATOM	1154	CD2	TRP	A	163	41.779	48.093	7.794	1.00	0.00
ATOM	1155	CE2	TRP	A	163	42.824	48.062	6.848	1.00	0.00
ATOM	1156	CE3	TRP	A	163	41.330	49.333	8.266	1.00	0.00
ATOM	1157	CD1	TRP	A	163	42.219	45.956	7.284	1.00	0.00
ATOM	1158	NE1	TRP	A	163	43.076	46.745	6.555	1.00	0.00
ATOM	1159	CZ2	TRP	A	163	43.434	49.231	6.358	1.00	0.00
ATOM	1160	CZ3	TRP	A	163	41.935	50.498	7.778	1.00	0.00
ATOM	1161	CH2	TRP	A	163	42.975	50.434	6.833	1.00	0.00
ATOM	1162	C	TRP	A	163	42.390	46.625	10.610	1.00	0.00
ATOM	1163	O	TRP	A	163	43.534	46.319	10.297	1.00	0.00
ATOM	1164	N	ALA	A	164	42.092	47.776	11.203	1.00	0.00
ATOM	1165	CA	ALA	A	164	43.124	48.755	11.543	1.00	0.00
ATOM	1166	CB	ALA	A	164	42.451	50.075	11.985	1.00	0.00
ATOM	1167	C	ALA	A	164	44.110	48.250	12.625	1.00	0.00
ATOM	1168	O	ALA	A	164	45.325	48.424	12.502	1.00	0.00
ATOM	1169	N	TRP	A	165	43.588	47.630	13.677	1.00	0.00
ATOM	1170	CA	TRP	A	165	44.422	47.098	14.772	1.00	0.00
ATOM	1171	CB	TRP	A	165	43.532	46.438	15.837	1.00	0.00
ATOM	1172	CG	TRP	A	165	44.226	46.012	17.106	1.00	0.00

Figure 1A-22

ATOM	1173	CD2	TRP	A	165	44.844	44.739	17.367	1.00	0.00
ATOM	1174	CE2	TRP	A	165	45.348	44.781	18.693	1.00	0.00
ATOM	1175	CE3	TRP	A	165	45.021	43.572	16.612	1.00	0.00
ATOM	1176	CD1	TRP	A	165	44.377	46.752	18.254	1.00	0.00
ATOM	1177	NE1	TRP	A	165	45.049	46.014	19.210	1.00	0.00
ATOM	1178	CZ2	TRP	A	165	46.019	43.701	19.274	1.00	0.00
ATOM	1179	CZ3	TRP	A	165	45.693	42.492	17.192	1.00	0.00
ATOM	1180	CH2	TRP	A	165	46.185	42.568	18.512	1.00	0.00
ATOM	1181	C	TRP	A	165	45.445	46.080	14.262	1.00	0.00
ATOM	1182	O	TRP	A	165	46.640	46.253	14.469	1.00	0.00
ATOM	1183	N	GLU	A	166	44.963	45.032	13.591	1.00	0.00
ATOM	1184	CA	GLU	A	166	45.795	43.953	13.036	1.00	0.00
ATOM	1185	CB	GLU	A	166	44.884	42.832	12.505	1.00	0.00
ATOM	1186	CG	GLU	A	166	45.586	41.728	11.704	1.00	0.00
ATOM	1187	CD	GLU	A	166	46.604	40.928	12.533	1.00	0.00
ATOM	1188	OE1	GLU	A	166	46.507	40.925	13.774	1.00	0.00
ATOM	1189	OE2	GLU	A	166	47.493	40.285	11.944	1.00	0.00
ATOM	1190	C	GLU	A	166	46.738	44.393	11.920	1.00	0.00
ATOM	1191	O	GLU	A	166	47.897	43.941	11.850	1.00	0.00
ATOM	1192	N	SER	A	167	46.244	45.257	11.035	1.00	0.00
ATOM	1193	CA	SER	A	167	47.062	45.745	9.924	1.00	0.00
ATOM	1194	CB	SER	A	167	46.210	46.593	8.965	1.00	0.00
ATOM	1195	OG	SER	A	167	45.210	45.800	8.353	1.00	0.00
ATOM	1196	C	SER	A	167	48.248	46.574	10.430	1.00	0.00
ATOM	1197	O	SER	A	167	49.353	46.491	9.887	1.00	0.00
ATOM	1198	N	TRP	A	168	48.015	47.386	11.458	1.00	0.00
ATOM	1199	CA	TRP	A	168	49.089	48.197	12.016	1.00	0.00
ATOM	1200	CB	TRP	A	168	48.579	49.055	13.185	1.00	0.00
ATOM	1201	CG	TRP	A	168	49.642	49.920	13.785	1.00	0.00
ATOM	1202	CD2	TRP	A	168	50.458	50.875	13.100	1.00	0.00
ATOM	1203	CE2	TRP	A	168	51.322	51.455	14.060	1.00	0.00
ATOM	1204	CE3	TRP	A	168	50.546	51.297	11.770	1.00	0.00
ATOM	1205	CD1	TRP	A	168	50.031	49.956	15.098	1.00	0.00
ATOM	1206	NE1	TRP	A	168	51.041	50.876	15.270	1.00	0.00
ATOM	1207	CZ2	TRP	A	168	52.260	52.442	13.730	1.00	0.00
ATOM	1208	CZ3	TRP	A	168	51.480	52.281	11.435	1.00	0.00
ATOM	1209	CH2	TRP	A	168	52.324	52.840	12.416	1.00	0.00
ATOM	1210	C	TRP	A	168	50.163	47.249	12.517	1.00	0.00
ATOM	1211	O	TRP	A	168	51.322	47.397	12.183	1.00	0.00
ATOM	1212	N	ARG	A	169	49.766	46.249	13.298	1.00	0.00
ATOM	1213	CA	ARG	A	169	50.738	45.302	13.835	1.00	0.00
ATOM	1214	CB	ARG	A	169	50.101	44.523	14.991	1.00	0.00
ATOM	1215	CG	ARG	A	169	49.783	45.427	16.175	1.00	0.00
ATOM	1216	CD	ARG	A	169	48.841	44.797	17.161	1.00	0.00
ATOM	1217	NE	ARG	A	169	48.733	45.630	18.357	1.00	0.00
ATOM	1218	CZ	ARG	A	169	48.093	46.795	18.401	1.00	0.00
ATOM	1219	NH1	ARG	A	169	48.057	47.497	19.529	1.00	0.00
ATOM	1220	NH2	ARG	A	169	47.465	47.250	17.328	1.00	0.00
ATOM	1221	C	ARG	A	169	51.307	44.355	12.793	1.00	0.00
ATOM	1222	O	ARG	A	169	52.448	43.930	12.881	1.00	0.00
ATOM	1223	N	SER	A	170	50.513	44.031	11.787	1.00	0.00
ATOM	1224	CA	SER	A	170	50.987	43.120	10.767	1.00	0.00
ATOM	1225	CB	SER	A	170	49.808	42.490	10.036	1.00	0.00
ATOM	1226	OG	SER	A	170	50.255	41.307	9.408	1.00	0.00
ATOM	1227	C	SER	A	170	51.933	43.765	9.767	1.00	0.00
ATOM	1228	O	SER	A	170	52.935	43.165	9.395	1.00	0.00

Figure 1A-23

ATOM	1229	N	GLU	A	171	51.635	44.987	9.336	1.00	0.00
ATOM	1230	CA	GLU	A	171	52.504	45.656	8.372	1.00	0.00
ATOM	1231	CB	GLU	A	171	51.711	46.646	7.519	1.00	0.00
ATOM	1232	CG	GLU	A	171	51.279	46.085	6.184	1.00	0.00
ATOM	1233	CD	GLU	A	171	50.291	44.961	6.336	1.00	0.00
ATOM	1234	OE1	GLU	A	171	49.114	45.255	6.636	1.00	0.00
ATOM	1235	OE2	GLU	A	171	50.693	43.787	6.171	1.00	0.00
ATOM	1236	C	GLU	A	171	53.715	46.376	8.955	1.00	0.00
ATOM	1237	O	GLU	A	171	54.818	46.245	8.431	1.00	0.00
ATOM	1238	N	VAL	A	172	53.545	47.149	10.018	1.00	0.00
ATOM	1239	CA	VAL	A	172	54.709	47.836	10.543	1.00	0.00
ATOM	1240	CB	VAL	A	172	54.379	49.313	10.932	1.00	0.00
ATOM	1241	CG1	VAL	A	172	53.598	49.976	9.818	1.00	0.00
ATOM	1242	CG2	VAL	A	172	53.591	49.365	12.214	1.00	0.00
ATOM	1243	C	VAL	A	172	55.320	47.105	11.721	1.00	0.00
ATOM	1244	O	VAL	A	172	56.533	46.965	11.805	1.00	0.00
ATOM	1245	N	GLY	A	173	54.492	46.620	12.631	1.00	0.00
ATOM	1246	CA	GLY	A	173	55.031	45.920	13.786	1.00	0.00
ATOM	1247	C	GLY	A	173	56.038	44.864	13.393	1.00	0.00
ATOM	1248	O	GLY	A	173	57.115	44.756	13.981	1.00	0.00
ATOM	1249	N	LYS	A	174	55.698	44.076	12.381	1.00	0.00
ATOM	1250	CA	LYS	A	174	56.595	43.025	11.931	1.00	0.00
ATOM	1251	CB	LYS	A	174	55.914	42.150	10.880	1.00	0.00
ATOM	1252	CG	LYS	A	174	54.813	41.274	11.444	1.00	0.00
ATOM	1253	CD	LYS	A	174	54.345	40.323	10.380	1.00	0.00
ATOM	1254	CE	LYS	A	174	53.191	39.478	10.856	1.00	0.00
ATOM	1255	NZ	LYS	A	174	52.924	38.386	9.873	1.00	0.00
ATOM	1256	C	LYS	A	174	57.903	43.560	11.382	1.00	0.00
ATOM	1257	O	LYS	A	174	58.914	42.877	11.427	1.00	0.00
ATOM	1258	N	GLN	A	175	57.891	44.774	10.842	1.00	0.00
ATOM	1259	CA	GLN	A	175	59.123	45.347	10.320	1.00	0.00
ATOM	1260	CB	GLN	A	175	58.843	46.645	9.582	1.00	0.00
ATOM	1261	CG	GLN	A	175	57.988	46.502	8.340	1.00	0.00
ATOM	1262	CD	GLN	A	175	57.941	47.793	7.571	1.00	0.00
ATOM	1263	OE1	GLN	A	175	58.986	48.345	7.213	1.00	0.00
ATOM	1264	NE2	GLN	A	175	56.742	48.298	7.320	1.00	0.00
ATOM	1265	C	GLN	A	175	60.019	45.653	11.509	1.00	0.00
ATOM	1266	O	GLN	A	175	61.235	45.641	11.411	1.00	0.00
ATOM	1267	N	LEU	A	176	59.385	45.930	12.636	1.00	0.00
ATOM	1268	CA	LEU	A	176	60.086	46.271	13.847	1.00	0.00
ATOM	1269	CB	LEU	A	176	59.133	47.005	14.775	1.00	0.00
ATOM	1270	CG	LEU	A	176	59.187	48.530	14.869	1.00	0.00
ATOM	1271	CD1	LEU	A	176	59.936	49.141	13.713	1.00	0.00
ATOM	1272	CD2	LEU	A	176	57.765	49.047	14.946	1.00	0.00
ATOM	1273	C	LEU	A	176	60.675	45.078	14.578	1.00	0.00
ATOM	1274	O	LEU	A	176	61.640	45.225	15.316	1.00	0.00
ATOM	1275	N	ARG	A	177	60.096	43.899	14.382	1.00	0.00
ATOM	1276	CA	ARG	A	177	60.568	42.720	15.094	1.00	0.00
ATOM	1277	CB	ARG	A	177	59.805	41.472	14.634	1.00	0.00
ATOM	1278	CG	ARG	A	177	60.208	40.198	15.367	1.00	0.00
ATOM	1279	CD	ARG	A	177	59.943	40.266	16.873	1.00	0.00
ATOM	1280	NE	ARG	A	177	60.651	39.198	17.583	1.00	0.00
ATOM	1281	CZ	ARG	A	177	60.065	38.286	18.358	1.00	0.00
ATOM	1282	NH1	ARG	A	177	60.800	37.356	18.961	1.00	0.00
ATOM	1283	NH2	ARG	A	177	58.751	38.303	18.538	1.00	0.00
ATOM	1284	C	ARG	A	177	62.072	42.500	14.991	1.00	0.00

Figure 1A-24

ATOM	1285	O	ARG	A	177	62.757	42.417	16.010	1.00	0.00
ATOM	1286	N	PRO	A	178	62.610	42.418	13.761	1.00	0.00
ATOM	1287	CD	PRO	A	178	61.915	42.573	12.477	1.00	0.00
ATOM	1288	CA	PRO	A	178	64.044	42.208	13.539	1.00	0.00
ATOM	1289	CB	PRO	A	178	64.173	42.297	12.022	1.00	0.00
ATOM	1290	CG	PRO	A	178	62.855	41.900	11.544	1.00	0.00
ATOM	1291	C	PRO	A	178	64.904	43.270	14.222	1.00	0.00
ATOM	1292	O	PRO	A	178	65.893	42.958	14.888	1.00	0.00
ATOM	1293	N	LEU	A	179	64.524	44.528	14.018	1.00	0.00
ATOM	1294	CA	LEU	A	179	65.250	45.651	14.582	1.00	0.00
ATOM	1295	CB	LEU	A	179	64.674	46.969	14.041	1.00	0.00
ATOM	1296	CG	LEU	A	179	64.691	47.050	12.508	1.00	0.00
ATOM	1297	CD1	LEU	A	179	63.840	48.212	11.998	1.00	0.00
ATOM	1298	CD2	LEU	A	179	66.122	47.176	12.048	1.00	0.00
ATOM	1299	C	LEU	A	179	65.226	45.669	16.108	1.00	0.00
ATOM	1300	O	LEU	A	179	66.243	45.936	16.747	1.00	0.00
ATOM	1301	N	TYR	A	180	64.070	45.389	16.690	1.00	0.00
ATOM	1302	CA	TYR	A	180	63.939	45.407	18.142	1.00	0.00
ATOM	1303	CB	TYR	A	180	62.482	45.175	18.568	1.00	0.00
ATOM	1304	CG	TYR	A	180	62.190	45.754	19.935	1.00	0.00
ATOM	1305	CD1	TYR	A	180	62.205	47.129	20.136	1.00	0.00
ATOM	1306	CE1	TYR	A	180	62.013	47.679	21.397	1.00	0.00
ATOM	1307	CD2	TYR	A	180	61.972	44.929	21.035	1.00	0.00
ATOM	1308	CE2	TYR	A	180	61.785	45.466	22.318	1.00	0.00
ATOM	1309	CZ	TYR	A	180	61.806	46.840	22.491	1.00	0.00
ATOM	1310	OH	TYR	A	180	61.638	47.378	23.749	1.00	0.00
ATOM	1311	C	TYR	A	180	64.837	44.398	18.851	1.00	0.00
ATOM	1312	O	TYR	A	180	65.384	44.702	19.900	1.00	0.00
ATOM	1313	N	GLU	A	181	64.981	43.204	18.281	1.00	0.00
ATOM	1314	CA	GLU	A	181	65.823	42.166	18.880	1.00	0.00
ATOM	1315	CB	GLU	A	181	65.702	40.847	18.102	1.00	0.00
ATOM	1316	CG	GLU	A	181	64.313	40.224	18.162	1.00	0.00
ATOM	1317	CD	GLU	A	181	64.177	38.988	17.289	1.00	0.00
ATOM	1318	OE1	GLU	A	181	65.134	38.668	16.550	1.00	0.00
ATOM	1319	OE2	GLU	A	181	63.107	38.340	17.337	1.00	0.00
ATOM	1320	C	GLU	A	181	67.277	42.615	18.901	1.00	0.00
ATOM	1321	O	GLU	A	181	67.954	42.506	19.922	1.00	0.00
ATOM	1322	N	GLU	A	182	67.762	43.121	17.775	1.00	0.00
ATOM	1323	CA	GLU	A	182	69.134	43.588	17.731	1.00	0.00
ATOM	1324	CB	GLU	A	182	69.485	44.065	16.322	1.00	0.00
ATOM	1325	CG	GLU	A	182	70.975	44.239	16.087	1.00	0.00
ATOM	1326	CD	GLU	A	182	71.293	44.660	14.665	1.00	0.00
ATOM	1327	OE1	GLU	A	182	72.477	44.958	14.383	1.00	0.00
ATOM	1328	OE2	GLU	A	182	70.359	44.688	13.831	1.00	0.00
ATOM	1329	C	GLU	A	182	69.261	44.728	18.749	1.00	0.00
ATOM	1330	O	GLU	A	182	70.240	44.806	19.482	1.00	0.00
ATOM	1331	N	TYR	A	183	68.246	45.586	18.810	1.00	0.00
ATOM	1332	CA	TYR	A	183	68.218	46.709	19.744	1.00	0.00
ATOM	1333	CB	TYR	A	183	66.928	47.499	19.542	1.00	0.00
ATOM	1334	CG	TYR	A	183	66.437	48.309	20.735	1.00	0.00
ATOM	1335	CD1	TYR	A	183	65.625	47.716	21.721	1.00	0.00
ATOM	1336	CE1	TYR	A	183	65.107	48.456	22.771	1.00	0.00
ATOM	1337	CD2	TYR	A	183	66.717	49.671	20.847	1.00	0.00
ATOM	1338	CE2	TYR	A	183	66.189	50.437	21.912	1.00	0.00
ATOM	1339	CZ	TYR	A	183	65.389	49.827	22.864	1.00	0.00
ATOM	1340	OH	TYR	A	183	64.837	50.566	23.906	1.00	0.00

Figure 1A-25

ATOM	1341	C	TYR	A	183	68.400	46.349	21.221	1.00	0.00
ATOM	1342	O	TYR	A	183	69.173	46.996	21.907	1.00	0.00
ATOM	1343	N	VAL	A	184	67.693	45.341	21.725	1.00	0.00
ATOM	1344	CA	VAL	A	184	67.867	44.972	23.127	1.00	0.00
ATOM	1345	CB	VAL	A	184	66.851	43.873	23.593	1.00	0.00
ATOM	1346	CG1	VAL	A	184	65.436	44.429	23.602	1.00	0.00
ATOM	1347	CG2	VAL	A	184	66.927	42.700	22.709	1.00	0.00
ATOM	1348	C	VAL	A	184	69.291	44.467	23.370	1.00	0.00
ATOM	1349	O	VAL	A	184	69.907	44.805	24.384	1.00	0.00
ATOM	1350	N	VAL	A	185	69.808	43.664	22.437	1.00	0.00
ATOM	1351	CA	VAL	A	185	71.171	43.131	22.535	1.00	0.00
ATOM	1352	CB	VAL	A	185	71.587	42.351	21.240	1.00	0.00
ATOM	1353	CG1	VAL	A	185	73.062	42.031	21.270	1.00	0.00
ATOM	1354	CG2	VAL	A	185	70.810	41.046	21.130	1.00	0.00
ATOM	1355	C	VAL	A	185	72.139	44.290	22.730	1.00	0.00
ATOM	1356	O	VAL	A	185	72.865	44.357	23.721	1.00	0.00
ATOM	1357	N	LEU	A	186	72.121	45.214	21.780	1.00	0.00
ATOM	1358	CA	LEU	A	186	72.990	46.375	21.820	1.00	0.00
ATOM	1359	CB	LEU	A	186	72.789	47.207	20.548	1.00	0.00
ATOM	1360	CG	LEU	A	186	73.833	47.087	19.433	1.00	0.00
ATOM	1361	CD1	LEU	A	186	74.480	45.712	19.421	1.00	0.00
ATOM	1362	CD2	LEU	A	186	73.154	47.381	18.106	1.00	0.00
ATOM	1363	C	LEU	A	186	72.804	47.253	23.046	1.00	0.00
ATOM	1364	O	LEU	A	186	73.771	47.808	23.565	1.00	0.00
ATOM	1365	N	LYS	A	187	71.570	47.382	23.510	1.00	0.00
ATOM	1366	CA	LYS	A	187	71.265	48.215	24.672	1.00	0.00
ATOM	1367	CB	LYS	A	187	69.765	48.519	24.713	1.00	0.00
ATOM	1368	CG	LYS	A	187	69.405	50.006	24.850	1.00	0.00
ATOM	1369	CD	LYS	A	187	69.940	50.823	23.702	1.00	0.00
ATOM	1370	CE	LYS	A	187	69.080	52.067	23.391	1.00	0.00
ATOM	1371	NZ	LYS	A	187	69.260	53.255	24.277	1.00	0.00
ATOM	1372	C	LYS	A	187	71.689	47.556	25.985	1.00	0.00
ATOM	1373	O	LYS	A	187	72.129	48.238	26.917	1.00	0.00
ATOM	1374	N	ASN	A	188	71.530	46.237	26.068	1.00	0.00
ATOM	1375	CA	ASN	A	188	71.925	45.522	27.272	1.00	0.00
ATOM	1376	CB	ASN	A	188	71.481	44.061	27.233	1.00	0.00
ATOM	1377	CG	ASN	A	188	70.131	43.852	27.870	1.00	0.00
ATOM	1378	OD1	ASN	A	188	69.721	44.614	28.758	1.00	0.00
ATOM	1379	ND2	ASN	A	188	69.434	42.801	27.444	1.00	0.00
ATOM	1380	C	ASN	A	188	73.436	45.580	27.373	1.00	0.00
ATOM	1381	O	ASN	A	188	74.002	45.586	28.466	1.00	0.00
ATOM	1382	N	GLU	A	189	74.081	45.632	26.217	1.00	0.00
ATOM	1383	CA	GLU	A	189	75.530	45.698	26.155	1.00	0.00
ATOM	1384	CB	GLU	A	189	75.976	45.496	24.711	1.00	0.00
ATOM	1385	CG	GLU	A	189	77.391	45.025	24.548	1.00	0.00
ATOM	1386	CD	GLU	A	189	77.634	44.469	23.164	1.00	0.00
ATOM	1387	OE1	GLU	A	189	76.843	43.595	22.735	1.00	0.00
ATOM	1388	OE2	GLU	A	189	78.614	44.899	22.509	1.00	0.00
ATOM	1389	C	GLU	A	189	75.971	47.063	26.668	1.00	0.00
ATOM	1390	O	GLU	A	189	76.896	47.166	27.455	1.00	0.00
ATOM	1391	N	MET	A	190	75.297	48.118	26.221	1.00	0.00
ATOM	1392	CA	MET	A	190	75.631	49.453	26.674	1.00	0.00
ATOM	1393	CB	MET	A	190	74.701	50.494	26.030	1.00	0.00
ATOM	1394	CG	MET	A	190	74.759	51.892	26.648	1.00	0.00
ATOM	1395	SD	MET	A	190	73.342	52.245	27.738	1.00	0.00
ATOM	1396	CE	MET	A	190	74.069	52.267	29.321	1.00	0.00

Figure 1A-26

ATOM	1397	C	MET	A	190	75.478	49.470	28.182	1.00	0.00
ATOM	1398	O	MET	A	190	76.402	49.854	28.904	1.00	0.00
ATOM	1399	N	ALA	A	191	74.318	49.022	28.650	1.00	0.00
ATOM	1400	CA	ALA	A	191	74.004	48.995	30.072	1.00	0.00
ATOM	1401	CB	ALA	A	191	72.602	48.444	30.267	1.00	0.00
ATOM	1402	C	ALA	A	191	75.011	48.217	30.947	1.00	0.00
ATOM	1403	O	ALA	A	191	75.427	48.696	32.004	1.00	0.00
ATOM	1404	N	ARG	A	192	75.401	47.025	30.515	1.00	0.00
ATOM	1405	CA	ARG	A	192	76.350	46.227	31.286	1.00	0.00
ATOM	1406	CB	ARG	A	192	76.560	44.853	30.641	1.00	0.00
ATOM	1407	CG	ARG	A	192	75.380	43.899	30.785	1.00	0.00
ATOM	1408	CD	ARG	A	192	75.813	42.468	30.507	1.00	0.00
ATOM	1409	NE	ARG	A	192	76.303	42.288	29.141	1.00	0.00
ATOM	1410	CZ	ARG	A	192	75.515	42.082	28.088	1.00	0.00
ATOM	1411	NH1	ARG	A	192	76.038	41.932	26.879	1.00	0.00
ATOM	1412	NH2	ARG	A	192	74.200	42.015	28.245	1.00	0.00
ATOM	1413	C	ARG	A	192	77.692	46.949	31.406	1.00	0.00
ATOM	1414	O	ARG	A	192	78.225	47.114	32.506	1.00	0.00
ATOM	1415	N	ALA	A	193	78.222	47.394	30.271	1.00	0.00
ATOM	1416	CA	ALA	A	193	79.495	48.093	30.248	1.00	0.00
ATOM	1417	CB	ALA	A	193	79.872	48.427	28.831	1.00	0.00
ATOM	1418	C	ALA	A	193	79.451	49.358	31.087	1.00	0.00
ATOM	1419	O	ALA	A	193	80.489	49.941	31.390	1.00	0.00
ATOM	1420	N	ASN	A	194	78.245	49.778	31.454	1.00	0.00
ATOM	1421	CA	ASN	A	194	78.037	50.975	32.270	1.00	0.00
ATOM	1422	CB	ASN	A	194	76.836	51.768	31.748	1.00	0.00
ATOM	1423	CG	ASN	A	194	77.223	52.786	30.698	1.00	0.00
ATOM	1424	OD1	ASN	A	194	77.797	53.829	31.013	1.00	0.00
ATOM	1425	ND2	ASN	A	194	76.920	52.487	29.441	1.00	0.00
ATOM	1426	C	ASN	A	194	77.796	50.574	33.717	1.00	0.00
ATOM	1427	O	ASN	A	194	77.384	51.390	34.544	1.00	0.00
ATOM	1428	N	HIS	A	195	78.031	49.297	33.996	1.00	0.00
ATOM	1429	CA	HIS	A	195	77.896	48.735	35.332	1.00	0.00
ATOM	1430	CB	HIS	A	195	78.725	49.578	36.317	1.00	0.00
ATOM	1431	CG	HIS	A	195	80.117	49.837	35.830	1.00	0.00
ATOM	1432	CD2	HIS	A	195	81.071	48.984	35.382	1.00	0.00
ATOM	1433	ND1	HIS	A	195	80.602	51.109	35.601	1.00	0.00
ATOM	1434	CE1	HIS	A	195	81.786	51.028	35.021	1.00	0.00
ATOM	1435	NE2	HIS	A	195	82.093	49.750	34.875	1.00	0.00
ATOM	1436	C	HIS	A	195	76.471	48.527	35.833	1.00	0.00
ATOM	1437	O	HIS	A	195	76.170	48.714	37.017	1.00	0.00
ATOM	1438	N	TYR	A	196	75.596	48.132	34.918	1.00	0.00
ATOM	1439	CA	TYR	A	196	74.213	47.831	35.250	1.00	0.00
ATOM	1440	CB	TYR	A	196	73.251	48.792	34.534	1.00	0.00
ATOM	1441	CG	TYR	A	196	73.258	50.215	35.054	1.00	0.00
ATOM	1442	CD1	TYR	A	196	72.465	50.587	36.142	1.00	0.00
ATOM	1443	CE1	TYR	A	196	72.463	51.899	36.618	1.00	0.00
ATOM	1444	CD2	TYR	A	196	74.054	51.190	34.451	1.00	0.00
ATOM	1445	CE2	TYR	A	196	74.064	52.496	34.917	1.00	0.00
ATOM	1446	CZ	TYR	A	196	73.269	52.848	35.998	1.00	0.00
ATOM	1447	OH	TYR	A	196	73.292	54.145	36.451	1.00	0.00
ATOM	1448	C	TYR	A	196	73.971	46.405	34.760	1.00	0.00
ATOM	1449	O	TYR	A	196	74.686	45.906	33.884	1.00	0.00
ATOM	1450	N	GLU	A	197	72.961	45.751	35.319	1.00	0.00
ATOM	1451	CA	GLU	A	197	72.617	44.380	34.926	1.00	0.00
ATOM	1452	CB	GLU	A	197	71.552	43.826	35.868	1.00	0.00

Figure 1A-27

ATOM	1453	CG	GLU	A	197	71.948	43.828	37.326	1.00	0.00
ATOM	1454	CD	GLU	A	197	70.749	43.902	38.239	1.00	0.00
ATOM	1455	OE1	GLU	A	197	69.759	43.164	38.002	1.00	0.00
ATOM	1456	OE2	GLU	A	197	70.801	44.705	39.195	1.00	0.00
ATOM	1457	C	GLU	A	197	72.081	44.308	33.496	1.00	0.00
ATOM	1458	O	GLU	A	197	72.480	43.448	32.704	1.00	0.00
ATOM	1459	N	ASP	A	198	71.155	45.208	33.184	1.00	0.00
ATOM	1460	CA	ASP	A	198	70.531	45.260	31.868	1.00	0.00
ATOM	1461	CB	ASP	A	198	69.435	44.198	31.769	1.00	0.00
ATOM	1462	CG	ASP	A	198	68.485	44.237	32.946	1.00	0.00
ATOM	1463	OD1	ASP	A	198	68.477	43.262	33.731	1.00	0.00
ATOM	1464	OD2	ASP	A	198	67.749	45.244	33.092	1.00	0.00
ATOM	1465	C	ASP	A	198	69.936	46.645	31.614	1.00	0.00
ATOM	1466	O	ASP	A	198	69.849	47.477	32.525	1.00	0.00
ATOM	1467	N	TYR	A	199	69.502	46.875	30.378	1.00	0.00
ATOM	1468	CA	TYR	A	199	68.950	48.173	29.999	1.00	0.00
ATOM	1469	CB	TYR	A	199	68.525	48.143	28.530	1.00	0.00
ATOM	1470	CG	TYR	A	199	68.174	49.503	27.965	1.00	0.00
ATOM	1471	CD1	TYR	A	199	68.970	50.614	28.230	1.00	0.00
ATOM	1472	CE1	TYR	A	199	68.675	51.850	27.684	1.00	0.00
ATOM	1473	CD2	TYR	A	199	67.065	49.667	27.138	1.00	0.00
ATOM	1474	CE2	TYR	A	199	66.760	50.894	26.583	1.00	0.00
ATOM	1475	CZ	TYR	A	199	67.566	51.979	26.856	1.00	0.00
ATOM	1476	OH	TYR	A	199	67.289	53.179	26.274	1.00	0.00
ATOM	1477	C	TYR	A	199	67.801	48.628	30.905	1.00	0.00
ATOM	1478	O	TYR	A	199	67.691	49.811	31.227	1.00	0.00
ATOM	1479	N	GLY	A	200	66.970	47.687	31.344	1.00	0.00
ATOM	1480	CA	GLY	A	200	65.875	48.043	32.223	1.00	0.00
ATOM	1481	C	GLY	A	200	66.350	48.463	33.605	1.00	0.00
ATOM	1482	O	GLY	A	200	65.748	49.326	34.249	1.00	0.00
ATOM	1483	N	ASP	A	201	67.416	47.827	34.084	1.00	0.00
ATOM	1484	CA	ASP	A	201	67.981	48.164	35.386	1.00	0.00
ATOM	1485	CB	ASP	A	201	69.103	47.154	35.727	1.00	0.00
ATOM	1486	CG	ASP	A	201	69.841	47.490	37.018	1.00	0.00
ATOM	1487	OD1	ASP	A	201	69.194	47.699	38.070	1.00	0.00
ATOM	1488	OD2	ASP	A	201	71.084	47.542	36.976	1.00	0.00
ATOM	1489	C	ASP	A	201	68.528	49.598	35.243	1.00	0.00
ATOM	1490	O	ASP	A	201	68.441	50.411	36.151	1.00	0.00
ATOM	1491	N	TYR	A	202	69.085	49.882	34.073	1.00	0.00
ATOM	1492	CA	TYR	A	202	69.624	51.198	33.737	1.00	0.00
ATOM	1493	CB	TYR	A	202	70.113	51.170	32.282	1.00	0.00
ATOM	1494	CG	TYR	A	202	70.711	52.462	31.758	1.00	0.00
ATOM	1495	CD1	TYR	A	202	72.010	52.848	32.108	1.00	0.00
ATOM	1496	CE1	TYR	A	202	72.585	54.015	31.589	1.00	0.00
ATOM	1497	CD2	TYR	A	202	69.991	53.280	30.880	1.00	0.00
ATOM	1498	CE2	TYR	A	202	70.544	54.445	30.355	1.00	0.00
ATOM	1499	CZ	TYR	A	202	71.846	54.807	30.708	1.00	0.00
ATOM	1500	OH	TYR	A	202	72.421	55.929	30.145	1.00	0.00
ATOM	1501	C	TYR	A	202	68.548	52.287	33.917	1.00	0.00
ATOM	1502	O	TYR	A	202	68.806	53.329	34.524	1.00	0.00
ATOM	1503	N	TRP	A	203	67.343	52.042	33.399	1.00	0.00
ATOM	1504	CA	TRP	A	203	66.239	53.001	33.512	1.00	0.00
ATOM	1505	CB	TRP	A	203	65.020	52.538	32.684	1.00	0.00
ATOM	1506	CG	TRP	A	203	65.109	52.786	31.206	1.00	0.00
ATOM	1507	CD2	TRP	A	203	64.290	52.195	30.191	1.00	0.00
ATOM	1508	CE2	TRP	A	203	64.703	52.734	28.956	1.00	0.00

Figure 1A-28

ATOM	1509	CE3	TRP	A	203	63.244	51.260	30.208	1.00	0.00
ATOM	1510	CD1	TRP	A	203	65.960	53.643	30.561	1.00	0.00
ATOM	1511	NE1	TRP	A	203	65.722	53.615	29.211	1.00	0.00
ATOM	1512	CZ2	TRP	A	203	64.107	52.368	27.740	1.00	0.00
ATOM	1513	CZ3	TRP	A	203	62.650	50.893	28.999	1.00	0.00
ATOM	1514	CH2	TRP	A	203	63.088	51.449	27.782	1.00	0.00
ATOM	1515	C	TRP	A	203	65.763	53.231	34.942	1.00	0.00
ATOM	1516	O	TRP	A	203	65.409	54.357	35.324	1.00	0.00
ATOM	1517	N	ARG	A	204	65.685	52.152	35.715	1.00	0.00
ATOM	1518	CA	ARG	A	204	65.241	52.255	37.093	1.00	0.00
ATOM	1519	CB	ARG	A	204	65.076	50.855	37.705	1.00	0.00
ATOM	1520	CG	ARG	A	204	63.979	50.021	37.035	1.00	0.00
ATOM	1521	CD	ARG	A	204	63.703	48.703	37.775	1.00	0.00
ATOM	1522	NE	ARG	A	204	64.813	47.747	37.720	1.00	0.00
ATOM	1523	CZ	ARG	A	204	64.983	46.842	36.758	1.00	0.00
ATOM	1524	NH1	ARG	A	204	64.119	46.762	35.752	1.00	0.00
ATOM	1525	NH2	ARG	A	204	66.001	45.988	36.811	1.00	0.00
ATOM	1526	C	ARG	A	204	66.267	53.095	37.858	1.00	0.00
ATOM	1527	O	ARG	A	204	66.022	53.554	38.969	1.00	0.00
ATOM	1528	N	GLY	A	205	67.412	53.305	37.225	1.00	0.00
ATOM	1529	CA	GLY	A	205	68.454	54.123	37.806	1.00	0.00
ATOM	1530	C	GLY	A	205	67.982	55.538	38.116	1.00	0.00
ATOM	1531	O	GLY	A	205	68.653	56.245	38.885	1.00	0.00
ATOM	1532	N	ASP	A	206	66.843	55.962	37.548	1.00	0.00
ATOM	1533	CA	ASP	A	206	66.328	57.325	37.807	1.00	0.00
ATOM	1534	CB	ASP	A	206	65.238	57.722	36.802	1.00	0.00
ATOM	1535	CG	ASP	A	206	64.742	59.159	37.003	1.00	0.00
ATOM	1536	OD1	ASP	A	206	63.705	59.364	37.678	1.00	0.00
ATOM	1537	OD2	ASP	A	206	65.401	60.095	36.487	1.00	0.00
ATOM	1538	C	ASP	A	206	65.759	57.502	39.205	1.00	0.00
ATOM	1539	O	ASP	A	206	65.673	58.628	39.697	1.00	0.00
ATOM	1540	N	TYR	A	207	65.356	56.399	39.837	1.00	0.00
ATOM	1541	CA	TYR	A	207	64.792	56.457	41.181	1.00	0.00
ATOM	1542	CB	TYR	A	207	63.609	55.498	41.283	1.00	0.00
ATOM	1543	CG	TYR	A	207	62.518	55.778	40.275	1.00	0.00
ATOM	1544	CD1	TYR	A	207	62.560	55.224	38.993	1.00	0.00
ATOM	1545	CE1	TYR	A	207	61.568	55.515	38.052	1.00	0.00
ATOM	1546	CD2	TYR	A	207	61.463	56.622	40.596	1.00	0.00
ATOM	1547	CE2	TYR	A	207	60.468	56.919	39.674	1.00	0.00
ATOM	1548	CZ	TYR	A	207	60.526	56.365	38.406	1.00	0.00
ATOM	1549	OH	TYR	A	207	59.533	56.668	37.504	1.00	0.00
ATOM	1550	C	TYR	A	207	65.821	56.135	42.296	1.00	0.00
ATOM	1551	O	TYR	A	207	65.557	56.333	43.487	1.00	0.00
ATOM	1552	N	GLU	A	208	66.991	55.661	41.898	1.00	0.00
ATOM	1553	CA	GLU	A	208	68.026	55.309	42.852	1.00	0.00
ATOM	1554	CB	GLU	A	208	69.129	54.507	42.161	1.00	0.00
ATOM	1555	CG	GLU	A	208	70.348	54.301	43.027	1.00	0.00
ATOM	1556	CD	GLU	A	208	71.353	53.349	42.419	1.00	0.00
ATOM	1557	OE1	GLU	A	208	71.587	53.411	41.185	1.00	0.00
ATOM	1558	OE2	GLU	A	208	71.924	52.541	43.184	1.00	0.00
ATOM	1559	C	GLU	A	208	68.652	56.484	43.586	1.00	0.00
ATOM	1560	O	GLU	A	208	69.037	57.482	42.981	1.00	0.00
ATOM	1561	N	VAL	A	209	68.739	56.359	44.902	1.00	0.00
ATOM	1562	CA	VAL	A	209	69.358	57.384	45.715	1.00	0.00
ATOM	1563	CB	VAL	A	209	68.299	58.316	46.352	1.00	0.00
ATOM	1564	CG1	VAL	A	209	66.939	57.678	46.274	1.00	0.00

Figure 1A-29

ATOM	1565	CG2	VAL	A	209	68.681	58.649	47.799	1.00	0.00
ATOM	1566	C	VAL	A	209	70.205	56.675	46.774	1.00	0.00
ATOM	1567	O	VAL	A	209	69.733	55.746	47.441	1.00	0.00
ATOM	1568	N	ASN	A	210	71.461	57.100	46.901	1.00	0.00
ATOM	1569	CA	ASN	A	210	72.394	56.490	47.846	1.00	0.00
ATOM	1570	CB	ASN	A	210	73.398	55.635	47.081	1.00	0.00
ATOM	1571	CG	ASN	A	210	72.743	54.457	46.390	1.00	0.00
ATOM	1572	OD1	ASN	A	210	73.393	53.701	45.669	1.00	0.00
ATOM	1573	ND2	ASN	A	210	71.442	54.293	46.610	1.00	0.00
ATOM	1574	C	ASN	A	210	73.160	57.460	48.739	1.00	0.00
ATOM	1575	O	ASN	A	210	73.088	58.686	48.575	1.00	0.00
ATOM	1576	N	GLY	A	211	73.899	56.887	49.688	1.00	0.00
ATOM	1577	CA	GLY	A	211	74.700	57.684	50.603	1.00	0.00
ATOM	1578	C	GLY	A	211	73.915	58.698	51.406	1.00	0.00
ATOM	1579	O	GLY	A	211	74.436	59.748	51.776	1.00	0.00
ATOM	1580	N	VAL	A	212	72.650	58.395	51.664	1.00	0.00
ATOM	1581	CA	VAL	A	212	71.797	59.280	52.445	1.00	0.00
ATOM	1582	CB	VAL	A	212	70.882	60.139	51.551	1.00	0.00
ATOM	1583	CG1	VAL	A	212	70.067	61.095	52.411	1.00	0.00
ATOM	1584	CG2	VAL	A	212	71.715	60.910	50.543	1.00	0.00
ATOM	1585	C	VAL	A	212	70.940	58.391	53.332	1.00	0.00
ATOM	1586	O	VAL	A	212	69.953	57.818	52.884	1.00	0.00
ATOM	1587	N	ASP	A	213	71.335	58.281	54.595	1.00	0.00
ATOM	1588	CA	ASP	A	213	70.640	57.447	55.568	1.00	0.00
ATOM	1589	CB	ASP	A	213	71.404	57.496	56.891	1.00	0.00
ATOM	1590	CG	ASP	A	213	72.886	57.222	56.709	1.00	0.00
ATOM	1591	OD1	ASP	A	213	73.345	56.125	57.108	1.00	0.00
ATOM	1592	OD2	ASP	A	213	73.586	58.105	56.150	1.00	0.00
ATOM	1593	C	ASP	A	213	69.181	57.843	55.793	1.00	0.00
ATOM	1594	O	ASP	A	213	68.878	58.987	56.137	1.00	0.00
ATOM	1595	N	GLY	A	214	68.278	56.887	55.601	1.00	0.00
ATOM	1596	CA	GLY	A	214	66.868	57.161	55.800	1.00	0.00
ATOM	1597	C	GLY	A	214	66.095	57.528	54.541	1.00	0.00
ATOM	1598	O	GLY	A	214	64.875	57.674	54.587	1.00	0.00
ATOM	1599	N	TYR	A	215	66.789	57.677	53.418	1.00	0.00
ATOM	1600	CA	TYR	A	215	66.124	58.036	52.174	1.00	0.00
ATOM	1601	CB	TYR	A	215	66.271	59.533	51.913	1.00	0.00
ATOM	1602	CG	TYR	A	215	65.634	60.394	52.970	1.00	0.00
ATOM	1603	CD1	TYR	A	215	64.257	60.608	52.992	1.00	0.00
ATOM	1604	CE1	TYR	A	215	63.670	61.421	53.967	1.00	0.00
ATOM	1605	CD2	TYR	A	215	66.416	61.013	53.959	1.00	0.00
ATOM	1606	CE2	TYR	A	215	65.838	61.831	54.944	1.00	0.00
ATOM	1607	CZ	TYR	A	215	64.474	62.030	54.937	1.00	0.00
ATOM	1608	OH	TYR	A	215	63.919	62.862	55.874	1.00	0.00
ATOM	1609	C	TYR	A	215	66.682	57.260	50.994	1.00	0.00
ATOM	1610	O	TYR	A	215	66.337	57.542	49.847	1.00	0.00
ATOM	1611	N	ASP	A	216	67.550	56.291	51.269	1.00	0.00
ATOM	1612	CA	ASP	A	216	68.127	55.487	50.204	1.00	0.00
ATOM	1613	CB	ASP	A	216	69.194	54.543	50.756	1.00	0.00
ATOM	1614	CG	ASP	A	216	70.545	55.220	50.902	1.00	0.00
ATOM	1615	OD1	ASP	A	216	71.531	54.542	51.267	1.00	0.00
ATOM	1616	OD2	ASP	A	216	70.624	56.436	50.645	1.00	0.00
ATOM	1617	C	ASP	A	216	67.040	54.693	49.477	1.00	0.00
ATOM	1618	O	ASP	A	216	65.973	54.434	50.026	1.00	0.00
ATOM	1619	N	TYR	A	217	67.313	54.311	48.239	1.00	0.00
ATOM	1620	CA	TYR	A	217	66.330	53.584	47.462	1.00	0.00

Figure 1A-30

ATOM	1621	CB	TYR	A	217	65.339	54.575	46.832	1.00	0.00
ATOM	1622	CG	TYR	A	217	64.087	53.924	46.285	1.00	0.00
ATOM	1623	CD1	TYR	A	217	62.967	53.742	47.085	1.00	0.00
ATOM	1624	CE1	TYR	A	217	61.827	53.109	46.590	1.00	0.00
ATOM	1625	CD2	TYR	A	217	64.042	53.460	44.977	1.00	0.00
ATOM	1626	CE2	TYR	A	217	62.912	52.823	44.476	1.00	0.00
ATOM	1627	CZ	TYR	A	217	61.811	52.651	45.284	1.00	0.00
ATOM	1628	OH	TYR	A	217	60.704	52.003	44.775	1.00	0.00
ATOM	1629	C	TYR	A	217	67.020	52.777	46.386	1.00	0.00
ATOM	1630	O	TYR	A	217	67.801	53.296	45.597	1.00	0.00
ATOM	1631	N	SER	A	218	66.712	51.496	46.347	1.00	0.00
ATOM	1632	CA	SER	A	218	67.322	50.589	45.388	1.00	0.00
ATOM	1633	CB	SER	A	218	67.322	49.174	45.979	1.00	0.00
ATOM	1634	OG	SER	A	218	67.802	48.231	45.033	1.00	0.00
ATOM	1635	C	SER	A	218	66.621	50.575	44.020	1.00	0.00
ATOM	1636	O	SER	A	218	65.453	50.940	43.908	1.00	0.00
ATOM	1637	N	ARG	A	219	67.340	50.133	42.993	1.00	0.00
ATOM	1638	CA	ARG	A	219	66.777	50.056	41.653	1.00	0.00
ATOM	1639	CB	ARG	A	219	67.881	49.828	40.608	1.00	0.00
ATOM	1640	CG	ARG	A	219	68.871	50.965	40.515	1.00	0.00
ATOM	1641	CD	ARG	A	219	69.584	50.987	39.182	1.00	0.00
ATOM	1642	NE	ARG	A	219	70.592	49.939	39.040	1.00	0.00
ATOM	1643	CZ	ARG	A	219	71.842	50.033	39.494	1.00	0.00
ATOM	1644	NH1	ARG	A	219	72.256	51.128	40.127	1.00	0.00
ATOM	1645	NH2	ARG	A	219	72.685	49.032	39.299	1.00	0.00
ATOM	1646	C	ARG	A	219	65.753	48.923	41.590	1.00	0.00
ATOM	1647	O	ARG	A	219	64.708	49.057	40.940	1.00	0.00
ATOM	1648	N	GLY	A	220	66.057	47.813	42.269	1.00	0.00
ATOM	1649	CA	GLY	A	220	65.151	46.670	42.300	1.00	0.00
ATOM	1650	C	GLY	A	220	63.958	46.954	43.189	1.00	0.00
ATOM	1651	O	GLY	A	220	62.892	46.357	43.046	1.00	0.00
ATOM	1652	N	GLN	A	221	64.140	47.885	44.115	1.00	0.00
ATOM	1653	CA	GLN	A	221	63.089	48.278	45.041	1.00	0.00
ATOM	1654	CB	GLN	A	221	63.670	49.276	46.047	1.00	0.00
ATOM	1655	CG	GLN	A	221	62.833	49.551	47.273	1.00	0.00
ATOM	1656	CD	GLN	A	221	63.605	50.333	48.335	1.00	0.00
ATOM	1657	OE1	GLN	A	221	64.806	50.103	48.556	1.00	0.00
ATOM	1658	NE2	GLN	A	221	62.916	51.249	49.010	1.00	0.00
ATOM	1659	C	GLN	A	221	61.912	48.908	44.276	1.00	0.00
ATOM	1660	O	GLN	A	221	60.776	48.884	44.749	1.00	0.00
ATOM	1661	N	LEU	A	222	62.196	49.490	43.106	1.00	0.00
ATOM	1662	CA	LEU	A	222	61.160	50.107	42.272	1.00	0.00
ATOM	1663	CB	LEU	A	222	61.771	50.766	41.025	1.00	0.00
ATOM	1664	CG	LEU	A	222	60.761	51.401	40.052	1.00	0.00
ATOM	1665	CD1	LEU	A	222	60.103	52.618	40.707	1.00	0.00
ATOM	1666	CD2	LEU	A	222	61.463	51.816	38.776	1.00	0.00
ATOM	1667	C	LEU	A	222	60.193	49.027	41.819	1.00	0.00
ATOM	1668	O	LEU	A	222	58.984	49.173	41.915	1.00	0.00
ATOM	1669	N	ILE	A	223	60.737	47.934	41.314	1.00	0.00
ATOM	1670	CA	ILE	A	223	59.898	46.845	40.845	1.00	0.00
ATOM	1671	CB	ILE	A	223	60.719	45.630	40.374	1.00	0.00
ATOM	1672	CG2	ILE	A	223	59.771	44.566	39.822	1.00	0.00
ATOM	1673	CG1	ILE	A	223	61.737	46.054	39.320	1.00	0.00
ATOM	1674	CD1	ILE	A	223	62.553	44.908	38.743	1.00	0.00
ATOM	1675	C	ILE	A	223	58.931	46.341	41.899	1.00	0.00
ATOM	1676	O	ILE	A	223	57.797	46.006	41.568	1.00	0.00

Figure 1A-31

ATOM	1677	N	GLU	A	224	59.344	46.275	43.162	1.00	0.00
ATOM	1678	CA	GLU	A	224	58.420	45.764	44.171	1.00	0.00
ATOM	1679	CB	GLU	A	224	59.171	45.036	45.313	1.00	0.00
ATOM	1680	CG	GLU	A	224	60.135	45.856	46.156	1.00	0.00
ATOM	1681	CD	GLU	A	224	61.036	44.979	47.040	1.00	0.00
ATOM	1682	OE1	GLU	A	224	61.845	44.204	46.480	1.00	0.00
ATOM	1683	OE2	GLU	A	224	60.940	45.063	48.290	1.00	0.00
ATOM	1684	C	GLU	A	224	57.438	46.793	44.718	1.00	0.00
ATOM	1685	O	GLU	A	224	56.333	46.437	45.126	1.00	0.00
ATOM	1686	N	ASP	A	225	57.807	48.068	44.720	1.00	0.00
ATOM	1687	CA	ASP	A	225	56.864	49.071	45.201	1.00	0.00
ATOM	1688	CB	ASP	A	225	57.583	50.382	45.493	1.00	0.00
ATOM	1689	CG	ASP	A	225	58.570	50.241	46.629	1.00	0.00
ATOM	1690	OD1	ASP	A	225	58.282	49.448	47.553	1.00	0.00
ATOM	1691	OD2	ASP	A	225	59.614	50.915	46.608	1.00	0.00
ATOM	1692	C	ASP	A	225	55.770	49.272	44.154	1.00	0.00
ATOM	1693	O	ASP	A	225	54.628	49.601	44.486	1.00	0.00
ATOM	1694	N	VAL	A	226	56.130	49.062	42.889	1.00	0.00
ATOM	1695	CA	VAL	A	226	55.174	49.186	41.796	1.00	0.00
ATOM	1696	CB	VAL	A	226	55.910	49.177	40.393	1.00	0.00
ATOM	1697	CG1	VAL	A	226	54.928	48.891	39.273	1.00	0.00
ATOM	1698	CG2	VAL	A	226	56.569	50.543	40.141	1.00	0.00
ATOM	1699	C	VAL	A	226	54.189	48.015	41.923	1.00	0.00
ATOM	1700	O	VAL	A	226	52.978	48.205	42.010	1.00	0.00
ATOM	1701	N	GLU	A	227	54.713	46.802	41.970	1.00	0.00
ATOM	1702	CA	GLU	A	227	53.861	45.621	42.091	1.00	0.00
ATOM	1703	CB	GLU	A	227	54.718	44.367	41.991	1.00	0.00
ATOM	1704	CG	GLU	A	227	55.549	44.391	40.724	1.00	0.00
ATOM	1705	CD	GLU	A	227	56.331	43.128	40.488	1.00	0.00
ATOM	1706	OE1	GLU	A	227	56.841	42.555	41.478	1.00	0.00
ATOM	1707	OE2	GLU	A	227	56.454	42.725	39.306	1.00	0.00
ATOM	1708	C	GLU	A	227	53.026	45.606	43.358	1.00	0.00
ATOM	1709	O	GLU	A	227	51.891	45.147	43.338	1.00	0.00
ATOM	1710	N	HIS	A	228	53.567	46.131	44.453	1.00	0.00
ATOM	1711	CA	HIS	A	228	52.832	46.164	45.717	1.00	0.00
ATOM	1712	CB	HIS	A	228	53.779	46.502	46.887	1.00	0.00
ATOM	1713	CG	HIS	A	228	53.074	46.776	48.180	1.00	0.00
ATOM	1714	CD2	HIS	A	228	52.877	45.998	49.272	1.00	0.00
ATOM	1715	ND1	HIS	A	228	52.444	47.975	48.447	1.00	0.00
ATOM	1716	CE1	HIS	A	228	51.889	47.923	49.647	1.00	0.00
ATOM	1717	NE2	HIS	A	228	52.137	46.733	50.169	1.00	0.00
ATOM	1718	C	HIS	A	228	51.702	47.176	45.642	1.00	0.00
ATOM	1719	O	HIS	A	228	50.584	46.917	46.095	1.00	0.00
ATOM	1720	N	THR	A	229	51.989	48.337	45.075	1.00	0.00
ATOM	1721	CA	THR	A	229	50.961	49.360	44.936	1.00	0.00
ATOM	1722	CB	THR	A	229	51.588	50.713	44.530	1.00	0.00
ATOM	1723	OG1	THR	A	229	50.542	51.667	44.340	1.00	0.00
ATOM	1724	CG2	THR	A	229	52.395	50.581	43.232	1.00	0.00
ATOM	1725	C	THR	A	229	49.915	48.935	43.879	1.00	0.00
ATOM	1726	O	THR	A	229	48.731	49.237	43.999	1.00	0.00
ATOM	1727	N	PHE	A	230	50.354	48.217	42.854	1.00	0.00
ATOM	1728	CA	PHE	A	230	49.444	47.771	41.810	1.00	0.00
ATOM	1729	CB	PHE	A	230	50.227	47.116	40.670	1.00	0.00
ATOM	1730	CG	PHE	A	230	49.365	46.710	39.526	1.00	0.00
ATOM	1731	CD1	PHE	A	230	48.647	47.668	38.816	1.00	0.00
ATOM	1732	CD2	PHE	A	230	49.188	45.363	39.214	1.00	0.00

Figure 1A-32

ATOM	1733	CE1	PHE	A	230	47.757	47.298	37.815	1.00	0.00
ATOM	1734	CE2	PHE	A	230	48.293	44.979	38.211	1.00	0.00
ATOM	1735	CZ	PHE	A	230	47.577	45.948	37.513	1.00	0.00
ATOM	1736	C	PHE	A	230	48.383	46.805	42.368	1.00	0.00
ATOM	1737	O	PHE	A	230	47.207	46.873	41.984	1.00	0.00
ATOM	1738	N	GLU	A	231	48.795	45.924	43.285	1.00	0.00
ATOM	1739	CA	GLU	A	231	47.876	44.970	43.919	1.00	0.00
ATOM	1740	CB	GLU	A	231	48.585	44.158	45.003	1.00	0.00
ATOM	1741	CG	GLU	A	231	49.464	43.030	44.490	1.00	0.00
ATOM	1742	CD	GLU	A	231	48.665	41.915	43.834	1.00	0.00
ATOM	1743	OE1	GLU	A	231	47.615	41.531	44.400	1.00	0.00
ATOM	1744	OE2	GLU	A	231	49.094	41.417	42.766	1.00	0.00
ATOM	1745	C	GLU	A	231	46.703	45.688	44.553	1.00	0.00
ATOM	1746	O	GLU	A	231	45.562	45.250	44.436	1.00	0.00
ATOM	1747	N	GLU	A	232	46.986	46.789	45.235	1.00	0.00
ATOM	1748	CA	GLU	A	232	45.934	47.569	45.882	1.00	0.00
ATOM	1749	CB	GLU	A	232	46.553	48.640	46.785	1.00	0.00
ATOM	1750	CG	GLU	A	232	46.809	48.190	48.214	1.00	0.00
ATOM	1751	CD	GLU	A	232	47.561	49.227	49.026	1.00	0.00
ATOM	1752	OE1	GLU	A	232	48.780	49.399	48.783	1.00	0.00
ATOM	1753	OE2	GLU	A	232	46.934	49.870	49.896	1.00	0.00
ATOM	1754	C	GLU	A	232	44.993	48.251	44.897	1.00	0.00
ATOM	1755	O	GLU	A	232	43.889	48.637	45.258	1.00	0.00
ATOM	1756	N	ILE	A	233	45.438	48.412	43.658	1.00	0.00
ATOM	1757	CA	ILE	A	233	44.630	49.074	42.641	1.00	0.00
ATOM	1758	CB	ILE	A	233	45.562	49.809	41.622	1.00	0.00
ATOM	1759	CG2	ILE	A	233	45.726	48.991	40.364	1.00	0.00
ATOM	1760	CG1	ILE	A	233	44.987	51.172	41.266	1.00	0.00
ATOM	1761	CD1	ILE	A	233	43.718	51.104	40.453	1.00	0.00
ATOM	1762	C	ILE	A	233	43.710	48.084	41.915	1.00	0.00
ATOM	1763	O	ILE	A	233	42.670	48.461	41.389	1.00	0.00
ATOM	1764	N	LYS	A	234	44.095	46.814	41.913	1.00	0.00
ATOM	1765	CA	LYS	A	234	43.324	45.770	41.241	1.00	0.00
ATOM	1766	CB	LYS	A	234	43.910	44.387	41.550	1.00	0.00
ATOM	1767	CG	LYS	A	234	45.167	44.047	40.756	1.00	0.00
ATOM	1768	CD	LYS	A	234	45.671	42.620	41.068	1.00	0.00
ATOM	1769	CE	LYS	A	234	46.938	42.287	40.285	1.00	0.00
ATOM	1770	NZ	LYS	A	234	47.534	40.953	40.615	1.00	0.00
ATOM	1771	C	LYS	A	234	41.810	45.734	41.466	1.00	0.00
ATOM	1772	O	LYS	A	234	41.060	45.632	40.504	1.00	0.00
ATOM	1773	N	PRO	A	235	41.337	45.807	42.726	1.00	0.00
ATOM	1774	CD	PRO	A	235	42.042	45.785	44.023	1.00	0.00
ATOM	1775	CA	PRO	A	235	39.885	45.770	42.927	1.00	0.00
ATOM	1776	CB	PRO	A	235	39.738	45.884	44.449	1.00	0.00
ATOM	1777	CG	PRO	A	235	40.982	45.221	44.950	1.00	0.00
ATOM	1778	C	PRO	A	235	39.158	46.887	42.183	1.00	0.00
ATOM	1779	O	PRO	A	235	38.131	46.656	41.550	1.00	0.00
ATOM	1780	N	LEU	A	236	39.685	48.101	42.260	1.00	0.00
ATOM	1781	CA	LEU	A	236	39.062	49.215	41.567	1.00	0.00
ATOM	1782	CB	LEU	A	236	39.801	50.520	41.874	1.00	0.00
ATOM	1783	CG	LEU	A	236	39.349	51.706	41.022	1.00	0.00
ATOM	1784	CD1	LEU	A	236	37.896	52.055	41.340	1.00	0.00
ATOM	1785	CD2	LEU	A	236	40.253	52.888	41.287	1.00	0.00
ATOM	1786	C	LEU	A	236	39.073	48.964	40.055	1.00	0.00
ATOM	1787	O	LEU	A	236	38.076	49.184	39.376	1.00	0.00
ATOM	1788	N	TYR	A	237	40.198	48.501	39.530	1.00	0.00

Figure 1A-33

ATOM	1789	CA	TYR	A	237	40.299	48.244	38.098	1.00	0.00
ATOM	1790	CB	TYR	A	237	41.719	47.837	37.735	1.00	0.00
ATOM	1791	CG	TYR	A	237	41.891	47.554	36.262	1.00	0.00
ATOM	1792	CD1	TYR	A	237	41.693	48.558	35.318	1.00	0.00
ATOM	1793	CE1	TYR	A	237	41.811	48.300	33.959	1.00	0.00
ATOM	1794	CD2	TYR	A	237	42.213	46.279	35.811	1.00	0.00
ATOM	1795	CE2	TYR	A	237	42.330	46.008	34.455	1.00	0.00
ATOM	1796	CZ	TYR	A	237	42.129	47.026	33.530	1.00	0.00
ATOM	1797	OH	TYR	A	237	42.275	46.777	32.180	1.00	0.00
ATOM	1798	C	TYR	A	237	39.329	47.168	37.614	1.00	0.00
ATOM	1799	O	TYR	A	237	38.615	47.378	36.633	1.00	0.00
ATOM	1800	N	GLU	A	238	39.312	46.021	38.296	1.00	0.00
ATOM	1801	CA	GLU	A	238	38.414	44.913	37.958	1.00	0.00
ATOM	1802	CB	GLU	A	238	38.478	43.809	39.020	1.00	0.00
ATOM	1803	CG	GLU	A	238	39.780	43.078	39.100	1.00	0.00
ATOM	1804	CD	GLU	A	238	39.735	41.917	40.091	1.00	0.00
ATOM	1805	OE1	GLU	A	238	40.778	41.232	40.250	1.00	0.00
ATOM	1806	OE2	GLU	A	238	38.665	41.694	40.706	1.00	0.00
ATOM	1807	C	GLU	A	238	36.963	45.375	37.855	1.00	0.00
ATOM	1808	O	GLU	A	238	36.235	44.935	36.967	1.00	0.00
ATOM	1809	N	HIS	A	239	36.544	46.233	38.783	1.00	0.00
ATOM	1810	CA	HIS	A	239	35.185	46.752	38.796	1.00	0.00
ATOM	1811	CB	HIS	A	239	34.882	47.412	40.139	1.00	0.00
ATOM	1812	CG	HIS	A	239	34.466	46.439	41.195	1.00	0.00
ATOM	1813	CD2	HIS	A	239	35.151	45.892	42.223	1.00	0.00
ATOM	1814	ND1	HIS	A	239	33.219	45.854	41.211	1.00	0.00
ATOM	1815	CE1	HIS	A	239	33.154	44.985	42.204	1.00	0.00
ATOM	1816	NE2	HIS	A	239	34.315	44.989	42.833	1.00	0.00
ATOM	1817	C	HIS	A	239	34.951	47.750	37.674	1.00	0.00
ATOM	1818	O	HIS	A	239	33.833	47.889	37.161	1.00	0.00
ATOM	1819	N	LEU	A	240	36.010	48.448	37.299	1.00	0.00
ATOM	1820	CA	LEU	A	240	35.920	49.408	36.227	1.00	0.00
ATOM	1821	CB	LEU	A	240	37.171	50.295	36.235	1.00	0.00
ATOM	1822	CG	LEU	A	240	37.218	51.534	35.337	1.00	0.00
ATOM	1823	CD1	LEU	A	240	37.885	51.207	34.057	1.00	0.00
ATOM	1824	CD2	LEU	A	240	35.829	52.076	35.120	1.00	0.00
ATOM	1825	C	LEU	A	240	35.851	48.554	34.966	1.00	0.00
ATOM	1826	O	LEU	A	240	35.101	48.833	34.046	1.00	0.00
ATOM	1827	N	HIS	A	241	36.636	47.489	34.965	1.00	0.00
ATOM	1828	CA	HIS	A	241	36.711	46.561	33.853	1.00	0.00
ATOM	1829	CB	HIS	A	241	37.820	45.552	34.146	1.00	0.00
ATOM	1830	CG	HIS	A	241	37.983	44.501	33.097	1.00	0.00
ATOM	1831	CD2	HIS	A	241	38.988	44.265	32.224	1.00	0.00
ATOM	1832	ND1	HIS	A	241	37.046	43.513	32.881	1.00	0.00
ATOM	1833	CE1	HIS	A	241	37.469	42.713	31.920	1.00	0.00
ATOM	1834	NE2	HIS	A	241	38.646	43.146	31.505	1.00	0.00
ATOM	1835	C	HIS	A	241	35.376	45.852	33.603	1.00	0.00
ATOM	1836	O	HIS	A	241	34.933	45.748	32.459	1.00	0.00
ATOM	1837	N	ALA	A	242	34.745	45.378	34.679	1.00	0.00
ATOM	1838	CA	ALA	A	242	33.465	44.678	34.609	1.00	0.00
ATOM	1839	CB	ALA	A	242	33.103	44.105	35.975	1.00	0.00
ATOM	1840	C	ALA	A	242	32.367	45.611	34.143	1.00	0.00
ATOM	1841	O	ALA	A	242	31.465	45.215	33.415	1.00	0.00
ATOM	1842	N	TYR	A	243	32.440	46.860	34.566	1.00	0.00
ATOM	1843	CA	TYR	A	243	31.435	47.819	34.167	1.00	0.00
ATOM	1844	CB	TYR	A	243	31.502	49.060	35.063	1.00	0.00

Figure 1A-34

ATOM	1845	CG	TYR	A	243	30.655	50.217	34.584	1.00	0.00
ATOM	1846	CD1	TYR	A	243	29.286	50.261	34.838	1.00	0.00
ATOM	1847	CE1	TYR	A	243	28.491	51.327	34.372	1.00	0.00
ATOM	1848	CD2	TYR	A	243	31.223	51.259	33.855	1.00	0.00
ATOM	1849	CE2	TYR	A	243	30.448	52.322	33.386	1.00	0.00
ATOM	1850	CZ	TYR	A	243	29.084	52.348	33.647	1.00	0.00
ATOM	1851	OH	TYR	A	243	28.321	53.390	33.173	1.00	0.00
ATOM	1852	C	TYR	A	243	31.586	48.216	32.694	1.00	0.00
ATOM	1853	O	TYR	A	243	30.594	48.260	31.961	1.00	0.00
ATOM	1854	N	VAL	A	244	32.801	48.500	32.236	1.00	0.00
ATOM	1855	CA	VAL	A	244	32.903	48.893	30.842	1.00	0.00
ATOM	1856	CB	VAL	A	244	34.261	49.586	30.486	1.00	0.00
ATOM	1857	CG1	VAL	A	244	34.728	50.518	31.642	1.00	0.00
ATOM	1858	CG2	VAL	A	244	35.294	48.558	30.115	1.00	0.00
ATOM	1859	C	VAL	A	244	32.681	47.658	29.972	1.00	0.00
ATOM	1860	O	VAL	A	244	32.068	47.749	28.920	1.00	0.00
ATOM	1861	N	ARG	A	245	33.157	46.500	30.418	1.00	0.00
ATOM	1862	CA	ARG	A	245	32.952	45.276	29.647	1.00	0.00
ATOM	1863	CB	ARG	A	245	33.609	44.076	30.349	1.00	0.00
ATOM	1864	CG	ARG	A	245	32.657	43.062	30.915	1.00	0.00
ATOM	1865	CD	ARG	A	245	32.832	41.698	30.285	1.00	0.00
ATOM	1866	NE	ARG	A	245	34.000	40.979	30.774	1.00	0.00
ATOM	1867	CZ	ARG	A	245	34.220	40.657	32.047	1.00	0.00
ATOM	1868	NH1	ARG	A	245	35.319	39.994	32.389	1.00	0.00
ATOM	1869	NH2	ARG	A	245	33.355	41.001	32.978	1.00	0.00
ATOM	1870	C	ARG	A	245	31.450	45.022	29.410	1.00	0.00
ATOM	1871	O	ARG	A	245	31.061	44.520	28.354	1.00	0.00
ATOM	1872	N	ALA	A	246	30.605	45.371	30.381	1.00	0.00
ATOM	1873	CA	ALA	A	246	29.164	45.183	30.213	1.00	0.00
ATOM	1874	CB	ALA	A	246	28.456	45.274	31.555	1.00	0.00
ATOM	1875	C	ALA	A	246	28.590	46.223	29.243	1.00	0.00
ATOM	1876	O	ALA	A	246	27.647	45.941	28.497	1.00	0.00
ATOM	1877	N	LYS	A	247	29.163	47.424	29.258	1.00	0.00
ATOM	1878	CA	LYS	A	247	28.722	48.493	28.378	1.00	0.00
ATOM	1879	CB	LYS	A	247	29.325	49.829	28.813	1.00	0.00
ATOM	1880	CG	LYS	A	247	28.691	50.418	30.059	1.00	0.00
ATOM	1881	CD	LYS	A	247	27.272	50.888	29.784	1.00	0.00
ATOM	1882	CE	LYS	A	247	26.665	51.555	31.008	1.00	0.00
ATOM	1883	NZ	LYS	A	247	25.280	52.047	30.732	1.00	0.00
ATOM	1884	C	LYS	A	247	29.127	48.196	26.943	1.00	0.00
ATOM	1885	O	LYS	A	247	28.358	48.450	26.013	1.00	0.00
ATOM	1886	N	LEU	A	248	30.332	47.660	26.764	1.00	0.00
ATOM	1887	CA	LEU	A	248	30.827	47.327	25.432	1.00	0.00
ATOM	1888	CB	LEU	A	248	32.320	46.986	25.472	1.00	0.00
ATOM	1889	CG	LEU	A	248	33.330	48.131	25.643	1.00	0.00
ATOM	1890	CD1	LEU	A	248	34.742	47.558	25.761	1.00	0.00
ATOM	1891	CD2	LEU	A	248	33.239	49.087	24.456	1.00	0.00
ATOM	1892	C	LEU	A	248	30.045	46.158	24.826	1.00	0.00
ATOM	1893	O	LEU	A	248	30.052	45.965	23.605	1.00	0.00
ATOM	1894	N	MET	A	249	29.383	45.372	25.671	1.00	0.00
ATOM	1895	CA	MET	A	249	28.593	44.257	25.168	1.00	0.00
ATOM	1896	CB	MET	A	249	28.191	43.307	26.296	1.00	0.00
ATOM	1897	CG	MET	A	249	29.350	42.456	26.776	1.00	0.00
ATOM	1898	SD	MET	A	249	28.897	41.264	28.046	1.00	0.00
ATOM	1899	CE	MET	A	249	28.527	42.325	29.411	1.00	0.00
ATOM	1900	C	MET	A	249	27.359	44.796	24.457	1.00	0.00

Figure 1A-35

ATOM	1901	O	MET	A	249	26.919	44.230	23.461	1.00	0.00
ATOM	1902	N	ASN	A	250	26.813	45.901	24.950	1.00	0.00
ATOM	1903	CA	ASN	A	250	25.647	46.490	24.307	1.00	0.00
ATOM	1904	CB	ASN	A	250	25.001	47.571	25.192	1.00	0.00
ATOM	1905	CG	ASN	A	250	24.484	47.020	26.525	1.00	0.00
ATOM	1906	OD1	ASN	A	250	24.155	45.834	26.646	1.00	0.00
ATOM	1907	ND2	ASN	A	250	24.391	47.894	27.526	1.00	0.00
ATOM	1908	C	ASN	A	250	26.086	47.105	22.981	1.00	0.00
ATOM	1909	O	ASN	A	250	25.379	47.006	21.974	1.00	0.00
ATOM	1910	N	ALA	A	251	27.267	47.724	22.984	1.00	0.00
ATOM	1911	CA	ALA	A	251	27.815	48.369	21.787	1.00	0.00
ATOM	1912	CB	ALA	A	251	28.996	49.262	22.164	1.00	0.00
ATOM	1913	C	ALA	A	251	28.247	47.381	20.705	1.00	0.00
ATOM	1914	O	ALA	A	251	28.197	47.701	19.521	1.00	0.00
ATOM	1915	N	TYR	A	252	28.670	46.189	21.113	1.00	0.00
ATOM	1916	CA	TYR	A	252	29.128	45.158	20.183	1.00	0.00
ATOM	1917	CB	TYR	A	252	30.645	44.999	20.315	1.00	0.00
ATOM	1918	CG	TYR	A	252	31.419	46.247	19.939	1.00	0.00
ATOM	1919	CD1	TYR	A	252	31.535	46.647	18.611	1.00	0.00
ATOM	1920	CE1	TYR	A	252	32.230	47.807	18.266	1.00	0.00
ATOM	1921	CD2	TYR	A	252	32.019	47.045	20.923	1.00	0.00
ATOM	1922	CE2	TYR	A	252	32.718	48.211	20.587	1.00	0.00
ATOM	1923	CZ	TYR	A	252	32.822	48.585	19.260	1.00	0.00
ATOM	1924	OH	TYR	A	252	33.541	49.726	18.926	1.00	0.00
ATOM	1925	C	TYR	A	252	28.420	43.831	20.484	1.00	0.00
ATOM	1926	O	TYR	A	252	29.046	42.831	20.849	1.00	0.00
ATOM	1927	N	PRO	A	253	27.093	43.808	20.316	1.00	0.00
ATOM	1928	CD	PRO	A	253	26.296	44.882	19.697	1.00	0.00
ATOM	1929	CA	PRO	A	253	26.266	42.624	20.572	1.00	0.00
ATOM	1930	CB	PRO	A	253	24.940	42.986	19.916	1.00	0.00
ATOM	1931	CG	PRO	A	253	24.888	44.471	20.043	1.00	0.00
ATOM	1932	C	PRO	A	253	26.839	41.317	20.030	1.00	0.00
ATOM	1933	O	PRO	A	253	27.146	41.218	18.850	1.00	0.00
ATOM	1934	N	SER	A	254	26.977	40.330	20.913	1.00	0.00
ATOM	1935	CA	SER	A	254	27.478	39.001	20.573	1.00	0.00
ATOM	1936	CB	SER	A	254	26.621	38.401	19.454	1.00	0.00
ATOM	1937	OG	SER	A	254	25.328	38.072	19.950	1.00	0.00
ATOM	1938	C	SER	A	254	28.952	38.862	20.214	1.00	0.00
ATOM	1939	O	SER	A	254	29.379	37.836	19.691	1.00	0.00
ATOM	1940	N	TYR	A	255	29.738	39.883	20.504	1.00	0.00
ATOM	1941	CA	TYR	A	255	31.162	39.828	20.210	1.00	0.00
ATOM	1942	CB	TYR	A	255	31.619	41.135	19.537	1.00	0.00
ATOM	1943	CG	TYR	A	255	31.340	41.223	18.045	1.00	0.00
ATOM	1944	CD1	TYR	A	255	30.561	42.255	17.517	1.00	0.00
ATOM	1945	CE1	TYR	A	255	30.363	42.377	16.131	1.00	0.00
ATOM	1946	CD2	TYR	A	255	31.911	40.308	17.153	1.00	0.00
ATOM	1947	CE2	TYR	A	255	31.722	40.421	15.782	1.00	0.00
ATOM	1948	CZ	TYR	A	255	30.949	41.457	15.275	1.00	0.00
ATOM	1949	OH	TYR	A	255	30.784	41.577	13.907	1.00	0.00
ATOM	1950	C	TYR	A	255	31.995	39.603	21.466	1.00	0.00
ATOM	1951	O	TYR	A	255	33.124	39.134	21.378	1.00	0.00
ATOM	1952	N	ILE	A	256	31.432	39.911	22.633	1.00	0.00
ATOM	1953	CA	ILE	A	256	32.181	39.802	23.886	1.00	0.00
ATOM	1954	CB	ILE	A	256	32.392	41.211	24.487	1.00	0.00
ATOM	1955	CG2	ILE	A	256	33.194	41.118	25.786	1.00	0.00
ATOM	1956	CG1	ILE	A	256	33.108	42.097	23.470	1.00	0.00

Figure 1A-36

ATOM	1957	CD1	ILE	A	256	33.032	43.574	23.800	1.00	0.00
ATOM	1958	C	ILE	A	256	31.552	38.913	24.962	1.00	0.00
ATOM	1959	O	ILE	A	256	30.360	38.987	25.212	1.00	0.00
ATOM	1960	N	SER	A	257	32.376	38.095	25.606	1.00	0.00
ATOM	1961	CA	SER	A	257	31.927	37.196	26.665	1.00	0.00
ATOM	1962	CB	SER	A	257	32.936	36.063	26.822	1.00	0.00
ATOM	1963	OG	SER	A	257	32.695	35.312	28.000	1.00	0.00
ATOM	1964	C	SER	A	257	31.751	37.935	28.010	1.00	0.00
ATOM	1965	O	SER	A	257	32.523	38.831	28.352	1.00	0.00
ATOM	1966	N	PRO	A	258	30.719	37.570	28.781	1.00	0.00
ATOM	1967	CD	PRO	A	258	29.664	36.613	28.403	1.00	0.00
ATOM	1968	CA	PRO	A	258	30.425	38.181	30.085	1.00	0.00
ATOM	1969	CB	PRO	A	258	29.110	37.503	30.501	1.00	0.00
ATOM	1970	CG	PRO	A	258	28.479	37.122	29.179	1.00	0.00
ATOM	1971	C	PRO	A	258	31.521	37.927	31.105	1.00	0.00
ATOM	1972	O	PRO	A	258	31.596	38.601	32.138	1.00	0.00
ATOM	1973	N	ILE	A	259	32.356	36.934	30.832	1.00	0.00
ATOM	1974	CA	ILE	A	259	33.425	36.611	31.758	1.00	0.00
ATOM	1975	CB	ILE	A	259	33.312	35.160	32.257	1.00	0.00
ATOM	1976	CG2	ILE	A	259	31.939	34.930	32.883	1.00	0.00
ATOM	1977	CG1	ILE	A	259	33.582	34.197	31.094	1.00	0.00
ATOM	1978	CD1	ILE	A	259	34.023	32.806	31.535	1.00	0.00
ATOM	1979	C	ILE	A	259	34.812	36.767	31.146	1.00	0.00
ATOM	1980	O	ILE	A	259	35.820	36.546	31.827	1.00	0.00
ATOM	1981	N	GLY	A	260	34.867	37.152	29.875	1.00	0.00
ATOM	1982	CA	GLY	A	260	36.153	37.265	29.217	1.00	0.00
ATOM	1983	C	GLY	A	260	36.842	38.616	29.190	1.00	0.00
ATOM	1984	O	GLY	A	260	36.278	39.648	29.574	1.00	0.00
ATOM	1985	N	CYS	A	261	38.095	38.586	28.747	1.00	0.00
ATOM	1986	CA	CYS	A	261	38.897	39.786	28.600	1.00	0.00
ATOM	1987	CB	CYS	A	261	40.315	39.423	28.166	1.00	0.00
ATOM	1988	SG	CYS	A	261	41.321	38.567	29.419	1.00	0.00
ATOM	1989	C	CYS	A	261	38.260	40.648	27.506	1.00	0.00
ATOM	1990	O	CYS	A	261	37.462	40.165	26.694	1.00	0.00
ATOM	1991	N	LEU	A	262	38.623	41.923	27.493	1.00	0.00
ATOM	1992	CA	LEU	A	262	38.125	42.849	26.501	1.00	0.00
ATOM	1993	CB	LEU	A	262	38.259	44.282	27.009	1.00	0.00
ATOM	1994	CG	LEU	A	262	37.458	44.552	28.278	1.00	0.00
ATOM	1995	CD1	LEU	A	262	37.774	45.953	28.830	1.00	0.00
ATOM	1996	CD2	LEU	A	262	35.966	44.383	27.949	1.00	0.00
ATOM	1997	C	LEU	A	262	38.968	42.680	25.254	1.00	0.00
ATOM	1998	O	LEU	A	262	40.183	42.594	25.341	1.00	0.00
ATOM	1999	N	PRO	A	263	38.330	42.583	24.080	1.00	0.00
ATOM	2000	CD	PRO	A	263	36.903	42.317	23.822	1.00	0.00
ATOM	2001	CA	PRO	A	263	39.119	42.431	22.856	1.00	0.00
ATOM	2002	CB	PRO	A	263	38.047	42.286	21.779	1.00	0.00
ATOM	2003	CG	PRO	A	263	36.959	41.535	22.516	1.00	0.00
ATOM	2004	C	PRO	A	263	39.986	43.689	22.687	1.00	0.00
ATOM	2005	O	PRO	A	263	39.500	44.810	22.823	1.00	0.00
ATOM	2006	N	ALA	A	264	41.268	43.489	22.398	1.00	0.00
ATOM	2007	CA	ALA	A	264	42.227	44.582	22.251	1.00	0.00
ATOM	2008	CB	ALA	A	264	43.572	43.995	21.885	1.00	0.00
ATOM	2009	C	ALA	A	264	41.887	45.745	21.291	1.00	0.00
ATOM	2010	O	ALA	A	264	42.296	46.899	21.535	1.00	0.00
ATOM	2011	N	HIS	A	265	41.140	45.460	20.223	1.00	0.00
ATOM	2012	CA	HIS	A	265	40.796	46.487	19.231	1.00	0.00

Figure 1A-37

ATOM	2013	CB	HIS	A	265	40.642	45.838	17.847	1.00	0.00
ATOM	2014	CG	HIS	A	265	39.459	44.924	17.736	1.00	0.00
ATOM	2015	CD2	HIS	A	265	38.389	44.945	16.903	1.00	0.00
ATOM	2016	ND1	HIS	A	265	39.294	43.818	18.541	1.00	0.00
ATOM	2017	CE1	HIS	A	265	38.177	43.194	18.209	1.00	0.00
ATOM	2018	NE2	HIS	A	265	37.608	43.858	17.216	1.00	0.00
ATOM	2019	C	HIS	A	265	39.553	47.313	19.518	1.00	0.00
ATOM	2020	O	HIS	A	265	39.172	48.138	18.700	1.00	0.00
ATOM	2021	N	LEU	A	266	38.923	47.107	20.672	1.00	0.00
ATOM	2022	CA	LEU	A	266	37.707	47.841	21.008	1.00	0.00
ATOM	2023	CB	LEU	A	266	36.598	46.843	21.389	1.00	0.00
ATOM	2024	CG	LEU	A	266	36.286	45.689	20.413	1.00	0.00
ATOM	2025	CD1	LEU	A	266	35.149	44.811	20.954	1.00	0.00
ATOM	2026	CD2	LEU	A	266	35.899	46.252	19.066	1.00	0.00
ATOM	2027	C	LEU	A	266	37.855	48.854	22.152	1.00	0.00
ATOM	2028	O	LEU	A	266	36.854	49.280	22.718	1.00	0.00
ATOM	2029	N	LEU	A	267	39.077	49.272	22.475	1.00	0.00
ATOM	2030	CA	LEU	A	267	39.280	50.161	23.629	1.00	0.00
ATOM	2031	CB	LEU	A	267	40.467	49.658	24.437	1.00	0.00
ATOM	2032	CG	LEU	A	267	40.440	48.173	24.801	1.00	0.00
ATOM	2033	CD1	LEU	A	267	41.843	47.754	25.266	1.00	0.00
ATOM	2034	CD2	LEU	A	267	39.381	47.907	25.862	1.00	0.00
ATOM	2035	C	LEU	A	267	39.424	51.675	23.464	1.00	0.00
ATOM	2036	O	LEU	A	267	39.684	52.374	24.446	1.00	0.00
ATOM	2037	N	GLY	A	268	39.299	52.211	22.262	1.00	0.00
ATOM	2038	CA	GLY	A	268	39.392	53.658	22.192	1.00	0.00
ATOM	2039	C	GLY	A	268	40.636	54.265	21.597	1.00	0.00
ATOM	2040	O	GLY	A	268	40.652	55.451	21.300	1.00	0.00
ATOM	2041	N	ASP	A	269	41.699	53.489	21.484	1.00	0.00
ATOM	2042	CA	ASP	A	269	42.887	53.983	20.824	1.00	0.00
ATOM	2043	CB	ASP	A	269	43.777	54.901	21.723	1.00	0.00
ATOM	2044	CG	ASP	A	269	44.596	54.168	22.802	1.00	0.00
ATOM	2045	OD1	ASP	A	269	44.849	54.839	23.826	1.00	0.00
ATOM	2046	OD2	ASP	A	269	45.034	53.006	22.650	1.00	0.00
ATOM	2047	C	ASP	A	269	43.559	52.754	20.274	1.00	0.00
ATOM	2048	O	ASP	A	269	43.066	51.647	20.473	1.00	0.00
ATOM	2049	N	MET	A	270	44.652	52.928	19.564	1.00	0.00
ATOM	2050	CA	MET	A	270	45.284	51.797	18.923	1.00	0.00
ATOM	2051	CB	MET	A	270	46.386	52.319	18.004	1.00	0.00
ATOM	2052	CG	MET	A	270	47.110	51.241	17.165	1.00	0.00
ATOM	2053	SD	MET	A	270	45.981	50.329	16.077	1.00	0.00
ATOM	2054	CE	MET	A	270	46.206	51.283	14.585	1.00	0.00
ATOM	2055	C	MET	A	270	45.822	50.676	19.818	1.00	0.00
ATOM	2056	O	MET	A	270	46.090	49.571	19.328	1.00	0.00
ATOM	2057	N	TRP	A	271	45.930	50.929	21.120	1.00	0.00
ATOM	2058	CA	TRP	A	271	46.532	49.941	22.017	1.00	0.00
ATOM	2059	CB	TRP	A	271	47.932	50.417	22.433	1.00	0.00
ATOM	2060	CG	TRP	A	271	48.795	50.912	21.308	1.00	0.00
ATOM	2061	CD2	TRP	A	271	48.847	52.247	20.788	1.00	0.00
ATOM	2062	CE2	TRP	A	271	49.759	52.243	19.717	1.00	0.00
ATOM	2063	CE3	TRP	A	271	48.210	53.448	21.132	1.00	0.00
ATOM	2064	CD1	TRP	A	271	49.662	50.173	20.547	1.00	0.00
ATOM	2065	NE1	TRP	A	271	50.242	50.966	19.588	1.00	0.00
ATOM	2066	CZ2	TRP	A	271	50.053	53.394	18.979	1.00	0.00
ATOM	2067	CZ3	TRP	A	271	48.505	54.598	20.399	1.00	0.00
ATOM	2068	CH2	TRP	A	271	49.415	54.559	19.338	1.00	0.00

Figure 1A-38

ATOM	2069	C	TRP	A	271	45.742	49.695	23.290	1.00	0.00
ATOM	2070	O	TRP	A	271	45.932	48.675	23.960	1.00	0.00
ATOM	2071	N	GLY	A	272	44.851	50.621	23.619	1.00	0.00
ATOM	2072	CA	GLY	A	272	44.125	50.507	24.864	1.00	0.00
ATOM	2073	C	GLY	A	272	44.960	51.180	25.965	1.00	0.00
ATOM	2074	O	GLY	A	272	44.847	50.836	27.150	1.00	0.00
ATOM	2075	N	ARG	A	273	45.810	52.133	25.576	1.00	0.00
ATOM	2076	CA	ARG	A	273	46.639	52.850	26.532	1.00	0.00
ATOM	2077	CB	ARG	A	273	47.597	53.810	25.826	1.00	0.00
ATOM	2078	CG	ARG	A	273	48.584	54.433	26.786	1.00	0.00
ATOM	2079	CD	ARG	A	273	49.475	55.470	26.142	1.00	0.00
ATOM	2080	NE	ARG	A	273	50.299	56.110	27.160	1.00	0.00
ATOM	2081	CZ	ARG	A	273	50.942	57.254	26.999	1.00	0.00
ATOM	2082	NH1	ARG	A	273	51.669	57.738	27.998	1.00	0.00
ATOM	2083	NH2	ARG	A	273	50.857	57.917	25.850	1.00	0.00
ATOM	2084	C	ARG	A	273	45.746	53.630	27.476	1.00	0.00
ATOM	2085	O	ARG	A	273	45.990	53.675	28.697	1.00	0.00
ATOM	2086	N	PHE	A	274	44.712	54.249	26.908	1.00	0.00
ATOM	2087	CA	PHE	A	274	43.737	55.004	27.698	1.00	0.00
ATOM	2088	CB	PHE	A	274	43.882	56.506	27.455	1.00	0.00
ATOM	2089	CG	PHE	A	274	45.252	57.045	27.737	1.00	0.00
ATOM	2090	CD1	PHE	A	274	46.033	57.542	26.704	1.00	0.00
ATOM	2091	CD2	PHE	A	274	45.737	57.119	29.054	1.00	0.00
ATOM	2092	CE1	PHE	A	274	47.285	58.122	26.962	1.00	0.00
ATOM	2093	CE2	PHE	A	274	46.985	57.690	29.333	1.00	0.00
ATOM	2094	CZ	PHE	A	274	47.762	58.197	28.288	1.00	0.00
ATOM	2095	C	PHE	A	274	42.365	54.554	27.204	1.00	0.00
ATOM	2096	O	PHE	A	274	42.249	54.163	26.056	1.00	0.00
ATOM	2097	N	TRP	A	275	41.347	54.587	28.065	1.00	0.00
ATOM	2098	CA	TRP	A	275	39.993	54.193	27.674	1.00	0.00
ATOM	2099	CB	TRP	A	275	39.353	53.263	28.718	1.00	0.00
ATOM	2100	CG	TRP	A	275	39.964	51.906	28.795	1.00	0.00
ATOM	2101	CD2	TRP	A	275	39.645	50.872	29.741	1.00	0.00
ATOM	2102	CE2	TRP	A	275	40.468	49.761	29.440	1.00	0.00
ATOM	2103	CE3	TRP	A	275	38.744	50.775	30.808	1.00	0.00
ATOM	2104	CD1	TRP	A	275	40.938	51.392	27.981	1.00	0.00
ATOM	2105	NE1	TRP	A	275	41.246	50.106	28.364	1.00	0.00
ATOM	2106	CZ2	TRP	A	275	40.415	48.563	30.172	1.00	0.00
ATOM	2107	CZ3	TRP	A	275	38.690	49.577	31.537	1.00	0.00
ATOM	2108	CH2	TRP	A	275	39.522	48.490	31.210	1.00	0.00
ATOM	2109	C	TRP	A	275	39.138	55.446	27.511	1.00	0.00
ATOM	2110	O	TRP	A	275	37.908	55.378	27.398	1.00	0.00
ATOM	2111	N	THR	A	276	39.812	56.591	27.496	1.00	0.00
ATOM	2112	CA	THR	A	276	39.168	57.893	27.335	1.00	0.00
ATOM	2113	CB	THR	A	276	40.185	58.955	26.856	1.00	0.00
ATOM	2114	OG1	THR	A	276	41.398	58.842	27.608	1.00	0.00
ATOM	2115	CG2	THR	A	276	39.613	60.347	27.026	1.00	0.00
ATOM	2116	C	THR	A	276	38.028	57.903	26.310	1.00	0.00
ATOM	2117	O	THR	A	276	36.925	58.356	26.591	1.00	0.00
ATOM	2118	N	ASN	A	277	38.309	57.416	25.111	1.00	0.00
ATOM	2119	CA	ASN	A	277	37.306	57.426	24.046	1.00	0.00
ATOM	2120	CB	ASN	A	277	38.000	57.226	22.702	1.00	0.00
ATOM	2121	CG	ASN	A	277	39.060	58.285	22.446	1.00	0.00
ATOM	2122	OD1	ASN	A	277	40.143	58.002	21.909	1.00	0.00
ATOM	2123	ND2	ASN	A	277	38.755	59.512	22.832	1.00	0.00
ATOM	2124	C	ASN	A	277	36.143	56.453	24.200	1.00	0.00

Figure 1A-39

ATOM	2125	O	ASN	A	277	35.286	56.377	23.333	1.00	0.00
ATOM	2126	N	LEU	A	278	36.109	55.723	25.308	1.00	0.00
ATOM	2127	CA	LEU	A	278	35.027	54.788	25.583	1.00	0.00
ATOM	2128	CB	LEU	A	278	35.546	53.612	26.427	1.00	0.00
ATOM	2129	CG	LEU	A	278	35.769	52.239	25.783	1.00	0.00
ATOM	2130	CD1	LEU	A	278	36.203	52.397	24.343	1.00	0.00
ATOM	2131	CD2	LEU	A	278	36.772	51.440	26.586	1.00	0.00
ATOM	2132	C	LEU	A	278	33.954	55.529	26.364	1.00	0.00
ATOM	2133	O	LEU	A	278	32.988	54.927	26.832	1.00	0.00
ATOM	2134	N	TYR	A	279	34.106	56.839	26.500	1.00	0.00
ATOM	2135	CA	TYR	A	279	33.146	57.606	27.283	1.00	0.00
ATOM	2136	CB	TYR	A	279	33.646	59.035	27.497	1.00	0.00
ATOM	2137	CG	TYR	A	279	32.854	59.756	28.550	1.00	0.00
ATOM	2138	CD1	TYR	A	279	32.897	59.346	29.874	1.00	0.00
ATOM	2139	CE1	TYR	A	279	32.147	59.997	30.854	1.00	0.00
ATOM	2140	CD2	TYR	A	279	32.029	60.842	28.219	1.00	0.00
ATOM	2141	CE2	TYR	A	279	31.267	61.501	29.193	1.00	0.00
ATOM	2142	CZ	TYR	A	279	31.335	61.073	30.509	1.00	0.00
ATOM	2143	OH	TYR	A	279	30.606	61.718	31.488	1.00	0.00
ATOM	2144	C	TYR	A	279	31.711	57.636	26.754	1.00	0.00
ATOM	2145	O	TYR	A	279	30.764	57.470	27.521	1.00	0.00
ATOM	2146	N	SER	A	280	31.538	57.853	25.459	1.00	0.00
ATOM	2147	CA	SER	A	280	30.194	57.875	24.876	1.00	0.00
ATOM	2148	CB	SER	A	280	30.270	58.283	23.409	1.00	0.00
ATOM	2149	OG	SER	A	280	30.522	59.674	23.300	1.00	0.00
ATOM	2150	C	SER	A	280	29.478	56.520	24.985	1.00	0.00
ATOM	2151	O	SER	A	280	28.248	56.454	25.008	1.00	0.00
ATOM	2152	N	LEU	A	281	30.250	55.443	25.054	1.00	0.00
ATOM	2153	CA	LEU	A	281	29.686	54.113	25.160	1.00	0.00
ATOM	2154	CB	LEU	A	281	30.598	53.086	24.466	1.00	0.00
ATOM	2155	CG	LEU	A	281	31.203	53.322	23.074	1.00	0.00
ATOM	2156	CD1	LEU	A	281	32.215	54.482	23.102	1.00	0.00
ATOM	2157	CD2	LEU	A	281	31.919	52.047	22.624	1.00	0.00
ATOM	2158	C	LEU	A	281	29.521	53.690	26.622	1.00	0.00
ATOM	2159	O	LEU	A	281	28.822	52.714	26.908	1.00	0.00
ATOM	2160	N	THR	A	282	30.154	54.406	27.554	1.00	0.00
ATOM	2161	CA	THR	A	282	30.075	54.006	28.966	1.00	0.00
ATOM	2162	CB	THR	A	282	31.482	53.583	29.503	1.00	0.00
ATOM	2163	OG1	THR	A	282	32.411	54.666	29.340	1.00	0.00
ATOM	2164	CG2	THR	A	282	32.016	52.373	28.763	1.00	0.00
ATOM	2165	C	THR	A	282	29.504	55.027	29.945	1.00	0.00
ATOM	2166	O	THR	A	282	29.278	54.703	31.106	1.00	0.00
ATOM	2167	N	VAL	A	283	29.279	56.256	29.499	1.00	0.00
ATOM	2168	CA	VAL	A	283	28.758	57.288	30.394	1.00	0.00
ATOM	2169	CB	VAL	A	283	28.415	58.589	29.599	1.00	0.00
ATOM	2170	CG1	VAL	A	283	27.394	58.295	28.502	1.00	0.00
ATOM	2171	CG2	VAL	A	283	27.914	59.665	30.549	1.00	0.00
ATOM	2172	C	VAL	A	283	27.545	56.840	31.233	1.00	0.00
ATOM	2173	O	VAL	A	283	26.501	56.482	30.693	1.00	0.00
ATOM	2174	N	PRO	A	284	27.680	56.861	32.577	1.00	0.00
ATOM	2175	CD	PRO	A	284	28.912	57.263	33.283	1.00	0.00
ATOM	2176	CA	PRO	A	284	26.640	56.468	33.537	1.00	0.00
ATOM	2177	CB	PRO	A	284	27.286	56.778	34.886	1.00	0.00
ATOM	2178	CG	PRO	A	284	28.757	56.586	34.618	1.00	0.00
ATOM	2179	C	PRO	A	284	25.271	57.159	33.378	1.00	0.00
ATOM	2180	O	PRO	A	284	24.226	56.513	33.518	1.00	0.00

40/396

Figure 1A-40

ATOM	2181	N	PHE	A	285	25.276	58.466	33.118	1.00	0.00
ATOM	2182	CA	PHE	A	285	24.037	59.227	32.939	1.00	0.00
ATOM	2183	CB	PHE	A	285	23.689	60.016	34.210	1.00	0.00
ATOM	2184	CG	PHE	A	285	23.688	59.178	35.456	1.00	0.00
ATOM	2185	CD1	PHE	A	285	24.849	59.028	36.206	1.00	0.00
ATOM	2186	CD2	PHE	A	285	22.548	58.463	35.828	1.00	0.00
ATOM	2187	CE1	PHE	A	285	24.887	58.168	37.307	1.00	0.00
ATOM	2188	CE2	PHE	A	285	22.567	57.598	36.925	1.00	0.00
ATOM	2189	CZ	PHE	A	285	23.743	57.447	37.668	1.00	0.00
ATOM	2190	C	PHE	A	285	24.198	60.189	31.772	1.00	0.00
ATOM	2191	O	PHE	A	285	24.526	61.364	31.956	1.00	0.00
ATOM	2192	N	GLY	A	286	23.947	59.684	30.569	1.00	0.00
ATOM	2193	CA	GLY	A	286	24.085	60.489	29.367	1.00	0.00
ATOM	2194	C	GLY	A	286	23.237	61.741	29.235	1.00	0.00
ATOM	2195	O	GLY	A	286	23.509	62.581	28.376	1.00	0.00
ATOM	2196	N	GLN	A	287	22.221	61.881	30.078	1.00	0.00
ATOM	2197	CA	GLN	A	287	21.331	63.042	30.025	1.00	0.00
ATOM	2198	CB	GLN	A	287	19.977	62.695	30.646	1.00	0.00
ATOM	2199	CG	GLN	A	287	19.729	61.191	30.796	1.00	0.00
ATOM	2200	CD	GLN	A	287	20.627	60.545	31.848	1.00	0.00
ATOM	2201	OE1	GLN	A	287	20.610	59.330	32.032	1.00	0.00
ATOM	2202	NE2	GLN	A	287	21.407	61.361	32.542	1.00	0.00
ATOM	2203	C	GLN	A	287	21.915	64.254	30.738	1.00	0.00
ATOM	2204	O	GLN	A	287	21.743	65.389	30.289	1.00	0.00
ATOM	2205	N	LYS	A	288	22.595	64.010	31.856	1.00	0.00
ATOM	2206	CA	LYS	A	288	23.207	65.088	32.625	1.00	0.00
ATOM	2207	CB	LYS	A	288	23.852	64.536	33.901	1.00	0.00
ATOM	2208	CG	LYS	A	288	22.862	64.078	34.966	1.00	0.00
ATOM	2209	CD	LYS	A	288	22.169	65.264	35.629	1.00	0.00
ATOM	2210	CE	LYS	A	288	21.080	64.818	36.600	1.00	0.00
ATOM	2211	NZ	LYS	A	288	21.604	63.965	37.702	1.00	0.00
ATOM	2212	C	LYS	A	288	24.261	65.789	31.781	1.00	0.00
ATOM	2213	O	LYS	A	288	25.077	65.141	31.126	1.00	0.00
ATOM	2214	N	PRO	A	289	24.246	67.129	31.769	1.00	0.00
ATOM	2215	CD	PRO	A	289	23.181	68.008	32.276	1.00	0.00
ATOM	2216	CA	PRO	A	289	25.224	67.896	30.988	1.00	0.00
ATOM	2217	CB	PRO	A	289	24.680	69.326	31.049	1.00	0.00
ATOM	2218	CG	PRO	A	289	23.206	69.129	31.266	1.00	0.00
ATOM	2219	C	PRO	A	289	26.630	67.801	31.585	1.00	0.00
ATOM	2220	O	PRO	A	289	26.809	67.886	32.802	1.00	0.00
ATOM	2221	N	ASN	A	290	27.617	67.621	30.716	1.00	0.00
ATOM	2222	CA	ASN	A	290	29.009	67.535	31.129	1.00	0.00
ATOM	2223	CB	ASN	A	290	29.801	66.751	30.080	1.00	0.00
ATOM	2224	CG	ASN	A	290	31.272	66.617	30.428	1.00	0.00
ATOM	2225	OD1	ASN	A	290	31.644	65.895	31.358	1.00	0.00
ATOM	2226	ND2	ASN	A	290	32.119	67.313	29.678	1.00	0.00
ATOM	2227	C	ASN	A	290	29.532	68.970	31.226	1.00	0.00
ATOM	2228	O	ASN	A	290	29.590	69.679	30.217	1.00	0.00
ATOM	2229	N	ILE	A	291	29.896	69.399	32.434	1.00	0.00
ATOM	2230	CA	ILE	A	291	30.404	70.757	32.648	1.00	0.00
ATOM	2231	CB	ILE	A	291	31.091	70.896	34.029	1.00	0.00
ATOM	2232	CG2	ILE	A	291	31.674	72.293	34.178	1.00	0.00
ATOM	2233	CG1	ILE	A	291	30.081	70.633	35.148	1.00	0.00
ATOM	2234	CD1	ILE	A	291	30.647	70.800	36.542	1.00	0.00
ATOM	2235	C	ILE	A	291	31.402	71.167	31.570	1.00	0.00
ATOM	2236	O	ILE	A	291	32.416	70.504	31.363	1.00	0.00

Figure 1A-41

ATOM	2237	N	ASP	A	292	31.109	72.267	30.886	1.00	0.00
ATOM	2238	CA	ASP	A	292	31.974	72.758	29.820	1.00	0.00
ATOM	2239	CB	ASP	A	292	31.666	72.023	28.515	1.00	0.00
ATOM	2240	CG	ASP	A	292	32.496	72.528	27.361	1.00	0.00
ATOM	2241	OD1	ASP	A	292	32.450	71.913	26.276	1.00	0.00
ATOM	2242	OD2	ASP	A	292	33.195	73.547	27.540	1.00	0.00
ATOM	2243	C	ASP	A	292	31.794	74.259	29.620	1.00	0.00
ATOM	2244	O	ASP	A	292	30.846	74.697	28.969	1.00	0.00
ATOM	2245	N	VAL	A	293	32.725	75.037	30.164	1.00	0.00
ATOM	2246	CA	VAL	A	293	32.666	76.491	30.079	1.00	0.00
ATOM	2247	CB	VAL	A	293	33.384	77.126	31.294	1.00	0.00
ATOM	2248	CG1	VAL	A	293	33.199	78.633	31.281	1.00	0.00
ATOM	2249	CG2	VAL	A	293	32.840	76.541	32.589	1.00	0.00
ATOM	2250	C	VAL	A	293	33.258	77.091	28.797	1.00	0.00
ATOM	2251	O	VAL	A	293	33.392	78.305	28.688	1.00	0.00
ATOM	2252	N	THR	A	294	33.586	76.252	27.820	1.00	0.00
ATOM	2253	CA	THR	A	294	34.179	76.747	26.583	1.00	0.00
ATOM	2254	CB	THR	A	294	34.647	75.575	25.680	1.00	0.00
ATOM	2255	OG1	THR	A	294	35.380	76.094	24.564	1.00	0.00
ATOM	2256	CG2	THR	A	294	33.461	74.780	25.161	1.00	0.00
ATOM	2257	C	THR	A	294	33.243	77.663	25.792	1.00	0.00
ATOM	2258	O	THR	A	294	33.569	78.099	24.685	1.00	0.00
ATOM	2259	N	ASP	A	295	32.086	77.956	26.379	1.00	0.00
ATOM	2260	CA	ASP	A	295	31.081	78.817	25.759	1.00	0.00
ATOM	2261	CB	ASP	A	295	29.743	78.071	25.668	1.00	0.00
ATOM	2262	CG	ASP	A	295	29.806	76.863	24.723	1.00	0.00
ATOM	2263	OD1	ASP	A	295	29.848	77.080	23.491	1.00	0.00
ATOM	2264	OD2	ASP	A	295	29.829	75.701	25.212	1.00	0.00
ATOM	2265	C	ASP	A	295	30.928	80.089	26.582	1.00	0.00
ATOM	2266	O	ASP	A	295	30.753	81.179	26.036	1.00	0.00
ATOM	2267	N	ALA	A	296	31.014	79.942	27.902	1.00	0.00
ATOM	2268	CA	ALA	A	296	30.901	81.070	28.820	1.00	0.00
ATOM	2269	CB	ALA	A	296	30.738	80.566	30.244	1.00	0.00
ATOM	2270	C	ALA	A	296	32.139	81.958	28.714	1.00	0.00
ATOM	2271	O	ALA	A	296	32.105	83.134	29.088	1.00	0.00
ATOM	2272	N	MET	A	297	33.231	81.381	28.216	1.00	0.00
ATOM	2273	CA	MET	A	297	34.484	82.108	28.032	1.00	0.00
ATOM	2274	CB	MET	A	297	35.632	81.133	27.725	1.00	0.00
ATOM	2275	CG	MET	A	297	36.141	80.325	28.931	1.00	0.00
ATOM	2276	SD	MET	A	297	37.220	78.928	28.469	1.00	0.00
ATOM	2277	CE	MET	A	297	38.638	79.782	27.773	1.00	0.00
ATOM	2278	C	MET	A	297	34.279	83.054	26.854	1.00	0.00
ATOM	2279	O	MET	A	297	34.624	84.238	26.912	1.00	0.00
ATOM	2280	N	VAL	A	298	33.706	82.514	25.786	1.00	0.00
ATOM	2281	CA	VAL	A	298	33.432	83.288	24.585	1.00	0.00
ATOM	2282	CB	VAL	A	298	32.746	82.407	23.521	1.00	0.00
ATOM	2283	CG1	VAL	A	298	32.468	83.216	22.263	1.00	0.00
ATOM	2284	CG2	VAL	A	298	33.629	81.210	23.206	1.00	0.00
ATOM	2285	C	VAL	A	298	32.537	84.489	24.903	1.00	0.00
ATOM	2286	O	VAL	A	298	32.930	85.640	24.693	1.00	0.00
ATOM	2287	N	ASP	A	299	31.343	84.212	25.425	1.00	0.00
ATOM	2288	CA	ASP	A	299	30.379	85.259	25.769	1.00	0.00
ATOM	2289	CB	ASP	A	299	29.159	84.641	26.469	1.00	0.00
ATOM	2290	CG	ASP	A	299	28.081	85.676	26.809	1.00	0.00
ATOM	2291	OD1	ASP	A	299	28.046	86.164	27.967	1.00	0.00
ATOM	2292	OD2	ASP	A	299	27.271	86.007	25.909	1.00	0.00

Figure 1A-42

ATOM	2293	C	ASP	A	299	30.972	86.376	26.636	1.00	0.00
ATOM	2294	O	ASP	A	299	30.458	87.498	26.654	1.00	0.00
ATOM	2295	N	GLN	A	300	32.047	86.075	27.355	1.00	0.00
ATOM	2296	CA	GLN	A	300	32.676	87.085	28.194	1.00	0.00
ATOM	2297	CB	GLN	A	300	33.101	86.481	29.534	1.00	0.00
ATOM	2298	CG	GLN	A	300	31.948	85.867	30.313	1.00	0.00
ATOM	2299	CD	GLN	A	300	32.287	85.610	31.766	1.00	0.00
ATOM	2300	OE1	GLN	A	300	31.491	85.036	32.502	1.00	0.00
ATOM	2301	NE2	GLN	A	300	33.470	86.041	32.190	1.00	0.00
ATOM	2302	C	GLN	A	300	33.877	87.686	27.469	1.00	0.00
ATOM	2303	O	GLN	A	300	34.665	88.432	28.053	1.00	0.00
ATOM	2304	N	ALA	A	301	33.997	87.360	26.186	1.00	0.00
ATOM	2305	CA	ALA	A	301	35.080	87.866	25.359	1.00	0.00
ATOM	2306	CB	ALA	A	301	34.903	89.362	25.123	1.00	0.00
ATOM	2307	C	ALA	A	301	36.427	87.601	26.000	1.00	0.00
ATOM	2308	O	ALA	A	301	37.162	88.536	26.324	1.00	0.00
ATOM	2309	N	TRP	A	302	36.743	86.323	26.192	1.00	0.00
ATOM	2310	CA	TRP	A	302	38.015	85.923	26.785	1.00	0.00
ATOM	2311	CB	TRP	A	302	37.842	84.676	27.657	1.00	0.00
ATOM	2312	CG	TRP	A	302	37.479	84.973	29.082	1.00	0.00
ATOM	2313	CD2	TRP	A	302	37.967	84.300	30.249	1.00	0.00
ATOM	2314	CE2	TRP	A	302	37.317	84.874	31.364	1.00	0.00
ATOM	2315	CE3	TRP	A	302	38.890	83.267	30.462	1.00	0.00
ATOM	2316	CD1	TRP	A	302	36.584	85.902	29.523	1.00	0.00
ATOM	2317	NE1	TRP	A	302	36.480	85.849	30.892	1.00	0.00
ATOM	2318	CZ2	TRP	A	302	37.560	84.450	32.677	1.00	0.00
ATOM	2319	CZ3	TRP	A	302	39.133	82.845	31.772	1.00	0.00
ATOM	2320	CH2	TRP	A	302	38.467	83.438	32.861	1.00	0.00
ATOM	2321	C	TRP	A	302	39.014	85.629	25.688	1.00	0.00
ATOM	2322	O	TRP	A	302	38.647	85.151	24.617	1.00	0.00
ATOM	2323	N	ASP	A	303	40.279	85.922	25.962	1.00	0.00
ATOM	2324	CA	ASP	A	303	41.346	85.681	25.003	1.00	0.00
ATOM	2325	CB	ASP	A	303	41.771	86.996	24.329	1.00	0.00
ATOM	2326	CG	ASP	A	303	41.983	88.127	25.323	1.00	0.00
ATOM	2327	OD1	ASP	A	303	42.935	88.059	26.133	1.00	0.00
ATOM	2328	OD2	ASP	A	303	41.186	89.091	25.296	1.00	0.00
ATOM	2329	C	ASP	A	303	42.536	85.042	25.703	1.00	0.00
ATOM	2330	O	ASP	A	303	42.540	84.890	26.926	1.00	0.00
ATOM	2331	N	ALA	A	304	43.535	84.671	24.912	1.00	0.00
ATOM	2332	CA	ALA	A	304	44.743	84.049	25.417	1.00	0.00
ATOM	2333	CB	ALA	A	304	45.796	84.027	24.322	1.00	0.00
ATOM	2334	C	ALA	A	304	45.278	84.775	26.647	1.00	0.00
ATOM	2335	O	ALA	A	304	45.523	84.163	27.686	1.00	0.00
ATOM	2336	N	GLN	A	305	45.455	86.083	26.528	1.00	0.00
ATOM	2337	CA	GLN	A	305	45.976	86.883	27.631	1.00	0.00
ATOM	2338	CB	GLN	A	305	45.960	88.364	27.251	1.00	0.00
ATOM	2339	CG	GLN	A	305	46.901	88.719	26.113	1.00	0.00
ATOM	2340	CD	GLN	A	305	48.364	88.635	26.511	1.00	0.00
ATOM	2341	OE1	GLN	A	305	48.786	89.234	27.511	1.00	0.00
ATOM	2342	NE2	GLN	A	305	49.152	87.897	25.726	1.00	0.00
ATOM	2343	C	GLN	A	305	45.209	86.687	28.935	1.00	0.00
ATOM	2344	O	GLN	A	305	45.811	86.534	30.002	1.00	0.00
ATOM	2345	N	ARG	A	306	43.882	86.707	28.844	1.00	0.00
ATOM	2346	CA	ARG	A	306	43.030	86.539	30.014	1.00	0.00
ATOM	2347	CB	ARG	A	306	41.572	86.832	29.646	1.00	0.00
ATOM	2348	CG	ARG	A	306	40.593	86.689	30.802	1.00	0.00

Figure 1A-43

ATOM	2349	CD	ARG	A	306	40.902	87.667	31.924	1.00	0.00
ATOM	2350	NE	ARG	A	306	39.962	87.529	33.032	1.00	0.00
ATOM	2351	CZ	ARG	A	306	38.641	87.627	32.909	1.00	0.00
ATOM	2352	NH1	ARG	A	306	38.095	87.867	31.719	1.00	0.00
ATOM	2353	NH2	ARG	A	306	37.862	87.482	33.977	1.00	0.00
ATOM	2354	C	ARG	A	306	43.156	85.123	30.580	1.00	0.00
ATOM	2355	O	ARG	A	306	43.097	84.927	31.788	1.00	0.00
ATOM	2356	N	ILE	A	307	43.321	84.144	29.697	1.00	0.00
ATOM	2357	CA	ILE	A	307	43.477	82.756	30.112	1.00	0.00
ATOM	2358	CB	ILE	A	307	43.575	81.837	28.889	1.00	0.00
ATOM	2359	CG2	ILE	A	307	44.156	80.485	29.281	1.00	0.00
ATOM	2360	CG1	ILE	A	307	42.188	81.714	28.252	1.00	0.00
ATOM	2361	CD1	ILE	A	307	42.134	80.833	27.041	1.00	0.00
ATOM	2362	C	ILE	A	307	44.729	82.597	30.983	1.00	0.00
ATOM	2363	O	ILE	A	307	44.648	82.081	32.099	1.00	0.00
ATOM	2364	N	PHE	A	308	45.873	83.064	30.483	1.00	0.00
ATOM	2365	CA	PHE	A	308	47.136	82.973	31.221	1.00	0.00
ATOM	2366	CB	PHE	A	308	48.316	83.212	30.277	1.00	0.00
ATOM	2367	CG	PHE	A	308	48.639	82.030	29.411	1.00	0.00
ATOM	2368	CD1	PHE	A	308	49.555	81.068	29.837	1.00	0.00
ATOM	2369	CD2	PHE	A	308	48.001	81.851	28.186	1.00	0.00
ATOM	2370	CE1	PHE	A	308	49.832	79.939	29.056	1.00	0.00
ATOM	2371	CE2	PHE	A	308	48.266	80.734	27.401	1.00	0.00
ATOM	2372	CZ	PHE	A	308	49.186	79.771	27.837	1.00	0.00
ATOM	2373	C	PHE	A	308	47.208	83.937	32.400	1.00	0.00
ATOM	2374	O	PHE	A	308	47.932	83.698	33.372	1.00	0.00
ATOM	2375	N	LYS	A	309	46.453	85.023	32.320	1.00	0.00
ATOM	2376	CA	LYS	A	309	46.441	85.999	33.395	1.00	0.00
ATOM	2377	CB	LYS	A	309	45.785	87.299	32.926	1.00	0.00
ATOM	2378	CG	LYS	A	309	45.909	88.440	33.920	1.00	0.00
ATOM	2379	CD	LYS	A	309	46.852	89.523	33.411	1.00	0.00
ATOM	2380	CE	LYS	A	309	48.199	88.958	33.015	1.00	0.00
ATOM	2381	NZ	LYS	A	309	49.154	90.032	32.617	1.00	0.00
ATOM	2382	C	LYS	A	309	45.652	85.406	34.553	1.00	0.00
ATOM	2383	O	LYS	A	309	45.951	85.662	35.723	1.00	0.00
ATOM	2384	N	GLU	A	310	44.641	84.609	34.223	1.00	0.00
ATOM	2385	CA	GLU	A	310	43.823	83.971	35.250	1.00	0.00
ATOM	2386	CB	GLU	A	310	42.516	83.459	34.631	1.00	0.00
ATOM	2387	CG	GLU	A	310	41.326	83.445	35.584	1.00	0.00
ATOM	2388	CD	GLU	A	310	40.885	84.837	36.023	1.00	0.00
ATOM	2389	OE1	GLU	A	310	40.574	85.678	35.150	1.00	0.00
ATOM	2390	OE2	GLU	A	310	40.836	85.086	37.246	1.00	0.00
ATOM	2391	C	GLU	A	310	44.633	82.819	35.874	1.00	0.00
ATOM	2392	O	GLU	A	310	44.549	82.567	37.070	1.00	0.00
ATOM	2393	N	ALA	A	311	45.425	82.132	35.055	1.00	0.00
ATOM	2394	CA	ALA	A	311	46.274	81.050	35.543	1.00	0.00
ATOM	2395	CB	ALA	A	311	46.980	80.357	34.379	1.00	0.00
ATOM	2396	C	ALA	A	311	47.304	81.676	36.488	1.00	0.00
ATOM	2397	O	ALA	A	311	47.575	81.147	37.565	1.00	0.00
ATOM	2398	N	GLU	A	312	47.868	82.812	36.084	1.00	0.00
ATOM	2399	CA	GLU	A	312	48.853	83.504	36.907	1.00	0.00
ATOM	2400	CB	GLU	A	312	49.376	84.749	36.183	1.00	0.00
ATOM	2401	CG	GLU	A	312	50.347	85.600	37.007	1.00	0.00
ATOM	2402	CD	GLU	A	312	50.797	86.854	36.262	1.00	0.00
ATOM	2403	OE1	GLU	A	312	49.926	87.676	35.905	1.00	0.00
ATOM	2404	OE2	GLU	A	312	52.013	87.017	36.028	1.00	0.00

Figure 1A-44

ATOM	2405	C	GLU	A	312	48.238	83.906	38.240	1.00	0.00
ATOM	2406	O	GLU	A	312	48.887	83.810	39.291	1.00	0.00
ATOM	2407	N	LYS	A	313	46.987	84.349	38.201	1.00	0.00
ATOM	2408	CA	LYS	A	313	46.306	84.760	39.417	1.00	0.00
ATOM	2409	CB	LYS	A	313	44.980	85.447	39.078	1.00	0.00
ATOM	2410	CG	LYS	A	313	44.205	85.937	40.298	1.00	0.00
ATOM	2411	CD	LYS	A	313	43.031	86.840	39.911	1.00	0.00
ATOM	2412	CE	LYS	A	313	42.265	87.295	41.154	1.00	0.00
ATOM	2413	NZ	LYS	A	313	41.063	88.130	40.839	1.00	0.00
ATOM	2414	C	LYS	A	313	46.067	83.559	40.340	1.00	0.00
ATOM	2415	O	LYS	A	313	46.030	83.704	41.571	1.00	0.00
ATOM	2416	N	PHE	A	314	45.900	82.376	39.747	1.00	0.00
ATOM	2417	CA	PHE	A	314	45.679	81.166	40.529	1.00	0.00
ATOM	2418	CB	PHE	A	314	45.405	79.978	39.607	1.00	0.00
ATOM	2419	CG	PHE	A	314	45.562	78.637	40.281	1.00	0.00
ATOM	2420	CD1	PHE	A	314	44.591	78.160	41.151	1.00	0.00
ATOM	2421	CD2	PHE	A	314	46.693	77.859	40.046	1.00	0.00
ATOM	2422	CE1	PHE	A	314	44.737	76.923	41.779	1.00	0.00
ATOM	2423	CE2	PHE	A	314	46.853	76.625	40.665	1.00	0.00
ATOM	2424	CZ	PHE	A	314	45.871	76.154	41.534	1.00	0.00
ATOM	2425	C	PHE	A	314	46.883	80.850	41.413	1.00	0.00
ATOM	2426	O	PHE	A	314	46.725	80.520	42.583	1.00	0.00
ATOM	2427	N	PHE	A	315	48.085	80.950	40.852	1.00	0.00
ATOM	2428	CA	PHE	A	315	49.303	80.652	41.609	1.00	0.00
ATOM	2429	CB	PHE	A	315	50.487	80.523	40.656	1.00	0.00
ATOM	2430	CG	PHE	A	315	50.388	79.344	39.728	1.00	0.00
ATOM	2431	CD1	PHE	A	315	50.584	78.051	40.201	1.00	0.00
ATOM	2432	CD2	PHE	A	315	50.071	79.521	38.390	1.00	0.00
ATOM	2433	CE1	PHE	A	315	50.460	76.945	39.348	1.00	0.00
ATOM	2434	CE2	PHE	A	315	49.946	78.431	37.535	1.00	0.00
ATOM	2435	CZ	PHE	A	315	50.140	77.141	38.017	1.00	0.00
ATOM	2436	C	PHE	A	315	49.608	81.670	42.709	1.00	0.00
ATOM	2437	O	PHE	A	315	49.909	81.293	43.853	1.00	0.00
ATOM	2438	N	VAL	A	316	49.521	82.954	42.371	1.00	0.00
ATOM	2439	CA	VAL	A	316	49.763	84.014	43.344	1.00	0.00
ATOM	2440	CB	VAL	A	316	49.563	85.422	42.703	1.00	0.00
ATOM	2441	CG1	VAL	A	316	49.498	86.503	43.776	1.00	0.00
ATOM	2442	CG2	VAL	A	316	50.715	85.716	41.755	1.00	0.00
ATOM	2443	C	VAL	A	316	48.797	83.841	44.516	1.00	0.00
ATOM	2444	O	VAL	A	316	49.130	84.140	45.659	1.00	0.00
ATOM	2445	N	SER	A	317	47.604	83.334	44.232	1.00	0.00
ATOM	2446	CA	SER	A	317	46.606	83.136	45.275	1.00	0.00
ATOM	2447	CB	SER	A	317	45.280	82.666	44.675	1.00	0.00
ATOM	2448	OG	SER	A	317	45.324	81.285	44.378	1.00	0.00
ATOM	2449	C	SER	A	317	47.066	82.136	46.332	1.00	0.00
ATOM	2450	O	SER	A	317	46.528	82.124	47.437	1.00	0.00
ATOM	2451	N	VAL	A	318	48.043	81.288	46.005	1.00	0.00
ATOM	2452	CA	VAL	A	318	48.542	80.337	47.004	1.00	0.00
ATOM	2453	CB	VAL	A	318	48.481	78.859	46.513	1.00	0.00
ATOM	2454	CG1	VAL	A	318	47.042	78.456	46.256	1.00	0.00
ATOM	2455	CG2	VAL	A	318	49.328	78.675	45.272	1.00	0.00
ATOM	2456	C	VAL	A	318	49.976	80.649	47.454	1.00	0.00
ATOM	2457	O	VAL	A	318	50.658	79.792	48.033	1.00	0.00
ATOM	2458	N	GLY	A	319	50.432	81.870	47.176	1.00	0.00
ATOM	2459	CA	GLY	A	319	51.763	82.271	47.605	1.00	0.00
ATOM	2460	C	GLY	A	319	52.918	82.192	46.616	1.00	0.00

Figure 1A-45

ATOM	2461	O	GLY	A	319	54.054	82.552	46.965	1.00	0.00
ATOM	2462	N	LEU	A	320	52.659	81.717	45.401	1.00	0.00
ATOM	2463	CA	LEU	A	320	53.715	81.631	44.401	1.00	0.00
ATOM	2464	CB	LEU	A	320	53.405	80.521	43.385	1.00	0.00
ATOM	2465	CG	LEU	A	320	53.358	79.099	43.964	1.00	0.00
ATOM	2466	CD1	LEU	A	320	52.814	78.115	42.933	1.00	0.00
ATOM	2467	CD2	LEU	A	320	54.746	78.686	44.416	1.00	0.00
ATOM	2468	C	LEU	A	320	53.813	82.990	43.716	1.00	0.00
ATOM	2469	O	LEU	A	320	52.880	83.792	43.785	1.00	0.00
ATOM	2470	N	PRO	A	321	54.954	83.275	43.064	1.00	0.00
ATOM	2471	CD	PRO	A	321	56.192	82.471	43.116	1.00	0.00
ATOM	2472	CA	PRO	A	321	55.197	84.539	42.361	1.00	0.00
ATOM	2473	CB	PRO	A	321	56.714	84.559	42.218	1.00	0.00
ATOM	2474	CG	PRO	A	321	57.044	83.121	42.040	1.00	0.00
ATOM	2475	C	PRO	A	321	54.509	84.709	41.010	1.00	0.00
ATOM	2476	O	PRO	A	321	54.131	83.737	40.359	1.00	0.00
ATOM	2477	N	ASN	A	322	54.356	85.966	40.603	1.00	0.00
ATOM	2478	CA	ASN	A	322	53.752	86.314	39.319	1.00	0.00
ATOM	2479	CB	ASN	A	322	53.658	87.842	39.161	1.00	0.00
ATOM	2480	CG	ASN	A	322	52.356	88.423	39.688	1.00	0.00
ATOM	2481	OD1	ASN	A	322	51.273	88.121	39.178	1.00	0.00
ATOM	2482	ND2	ASN	A	322	52.457	89.277	40.701	1.00	0.00
ATOM	2483	C	ASN	A	322	54.697	85.797	38.250	1.00	0.00
ATOM	2484	O	ASN	A	322	55.853	85.489	38.534	1.00	0.00
ATOM	2485	N	MET	A	323	54.214	85.694	37.023	1.00	0.00
ATOM	2486	CA	MET	A	323	55.085	85.276	35.936	1.00	0.00
ATOM	2487	CB	MET	A	323	54.285	85.171	34.644	1.00	0.00
ATOM	2488	CG	MET	A	323	53.394	83.948	34.582	1.00	0.00
ATOM	2489	SD	MET	A	323	54.407	82.462	34.522	1.00	0.00
ATOM	2490	CE	MET	A	323	54.478	82.037	36.264	1.00	0.00
ATOM	2491	C	MET	A	323	56.115	86.404	35.827	1.00	0.00
ATOM	2492	O	MET	A	323	55.904	87.485	36.389	1.00	0.00
ATOM	2493	N	THR	A	324	57.229	86.177	35.140	1.00	0.00
ATOM	2494	CA	THR	A	324	58.212	87.244	35.021	1.00	0.00
ATOM	2495	CB	THR	A	324	59.634	86.737	34.758	1.00	0.00
ATOM	2496	OG1	THR	A	324	59.677	86.098	33.475	1.00	0.00
ATOM	2497	CG2	THR	A	324	60.092	85.794	35.860	1.00	0.00
ATOM	2498	C	THR	A	324	57.907	88.175	33.865	1.00	0.00
ATOM	2499	O	THR	A	324	57.150	87.843	32.947	1.00	0.00
ATOM	2500	N	GLN	A	325	58.517	89.352	33.932	1.00	0.00
ATOM	2501	CA	GLN	A	325	58.404	90.349	32.884	1.00	0.00
ATOM	2502	CB	GLN	A	325	59.038	91.663	33.352	1.00	0.00
ATOM	2503	CG	GLN	A	325	58.839	92.850	32.415	1.00	0.00
ATOM	2504	CD	GLN	A	325	59.394	92.606	31.025	1.00	0.00
ATOM	2505	OE1	GLN	A	325	60.568	92.255	30.859	1.00	0.00
ATOM	2506	NE2	GLN	A	325	58.551	92.798	30.011	1.00	0.00
ATOM	2507	C	GLN	A	325	59.270	89.691	31.825	1.00	0.00
ATOM	2508	O	GLN	A	325	60.394	89.285	32.107	1.00	0.00
ATOM	2509	N	GLY	A	326	58.773	89.563	30.610	1.00	0.00
ATOM	2510	CA	GLY	A	326	59.590	88.895	29.613	1.00	0.00
ATOM	2511	C	GLY	A	326	58.887	87.601	29.294	1.00	0.00
ATOM	2512	O	GLY	A	326	58.846	87.176	28.140	1.00	0.00
ATOM	2513	N	PHE	A	327	58.350	86.957	30.327	1.00	0.00
ATOM	2514	CA	PHE	A	327	57.578	85.753	30.101	1.00	0.00
ATOM	2515	CB	PHE	A	327	57.034	85.173	31.414	1.00	0.00
ATOM	2516	CG	PHE	A	327	55.843	84.276	31.218	1.00	0.00

Figure 1A-46

ATOM	2517	CD1	PHE	A	327	54.548	84.772	31.373	1.00	0.00
ATOM	2518	CD2	PHE	A	327	56.009	82.960	30.790	1.00	0.00
ATOM	2519	CE1	PHE	A	327	53.441	83.980	31.100	1.00	0.00
ATOM	2520	CE2	PHE	A	327	54.910	82.155	30.511	1.00	0.00
ATOM	2521	CZ	PHE	A	327	53.619	82.667	30.665	1.00	0.00
ATOM	2522	C	PHE	A	327	56.422	86.251	29.231	1.00	0.00
ATOM	2523	O	PHE	A	327	56.119	85.672	28.198	1.00	0.00
ATOM	2524	N	TRP	A	328	55.799	87.351	29.646	1.00	0.00
ATOM	2525	CA	TRP	A	328	54.690	87.933	28.885	1.00	0.00
ATOM	2526	CB	TRP	A	328	53.993	89.025	29.696	1.00	0.00
ATOM	2527	CG	TRP	A	328	53.270	88.517	30.895	1.00	0.00
ATOM	2528	CD2	TRP	A	328	52.051	87.765	30.906	1.00	0.00
ATOM	2529	CE2	TRP	A	328	51.735	87.502	32.257	1.00	0.00
ATOM	2530	CE3	TRP	A	328	51.193	87.288	29.906	1.00	0.00
ATOM	2531	CD1	TRP	A	328	53.636	88.672	32.197	1.00	0.00
ATOM	2532	NE1	TRP	A	328	52.719	88.068	33.024	1.00	0.00
ATOM	2533	CZ2	TRP	A	328	50.594	86.782	32.634	1.00	0.00
ATOM	2534	CZ3	TRP	A	328	50.059	86.574	30.279	1.00	0.00
ATOM	2535	CH2	TRP	A	328	49.770	86.329	31.630	1.00	0.00
ATOM	2536	C	TRP	A	328	55.128	88.523	27.543	1.00	0.00
ATOM	2537	O	TRP	A	328	54.368	88.510	26.569	1.00	0.00
ATOM	2538	N	GLU	A	329	56.354	89.036	27.493	1.00	0.00
ATOM	2539	CA	GLU	A	329	56.880	89.629	26.267	1.00	0.00
ATOM	2540	CB	GLU	A	329	57.996	90.623	26.598	1.00	0.00
ATOM	2541	CG	GLU	A	329	58.661	91.245	25.360	1.00	0.00
ATOM	2542	CD	GLU	A	329	57.772	92.256	24.623	1.00	0.00
ATOM	2543	OE1	GLU	A	329	56.542	92.024	24.509	1.00	0.00
ATOM	2544	OE2	GLU	A	329	58.316	93.280	24.143	1.00	0.00
ATOM	2545	C	GLU	A	329	57.409	88.601	25.270	1.00	0.00
ATOM	2546	O	GLU	A	329	57.128	88.679	24.073	1.00	0.00
ATOM	2547	N	ASN	A	330	58.165	87.630	25.766	1.00	0.00
ATOM	2548	CA	ASN	A	330	58.755	86.608	24.910	1.00	0.00
ATOM	2549	CB	ASN	A	330	60.040	86.101	25.555	1.00	0.00
ATOM	2550	CG	ASN	A	330	60.992	87.217	25.879	1.00	0.00
ATOM	2551	OD1	ASN	A	330	61.538	87.285	26.981	1.00	0.00
ATOM	2552	ND2	ASN	A	330	61.203	88.107	24.914	1.00	0.00
ATOM	2553	C	ASN	A	330	57.866	85.417	24.563	1.00	0.00
ATOM	2554	O	ASN	A	330	58.115	84.737	23.570	1.00	0.00
ATOM	2555	N	SER	A	331	56.844	85.157	25.375	1.00	0.00
ATOM	2556	CA	SER	A	331	55.945	84.024	25.138	1.00	0.00
ATOM	2557	CB	SER	A	331	55.007	83.795	26.339	1.00	0.00
ATOM	2558	OG	SER	A	331	55.652	83.206	27.451	1.00	0.00
ATOM	2559	C	SER	A	331	55.072	84.190	23.906	1.00	0.00
ATOM	2560	O	SER	A	331	54.609	85.289	23.599	1.00	0.00
ATOM	2561	N	MET	A	332	54.851	83.085	23.207	1.00	0.00
ATOM	2562	CA	MET	A	332	53.977	83.064	22.045	1.00	0.00
ATOM	2563	CB	MET	A	332	54.603	82.277	20.885	1.00	0.00
ATOM	2564	CG	MET	A	332	53.648	82.071	19.719	1.00	0.00
ATOM	2565	SD	MET	A	332	54.358	81.247	18.275	1.00	0.00
ATOM	2566	CE	MET	A	332	55.288	82.630	17.563	1.00	0.00
ATOM	2567	C	MET	A	332	52.728	82.342	22.547	1.00	0.00
ATOM	2568	O	MET	A	332	52.642	81.118	22.487	1.00	0.00
ATOM	2569	N	LEU	A	333	51.775	83.110	23.061	1.00	0.00
ATOM	2570	CA	LEU	A	333	50.532	82.568	23.598	1.00	0.00
ATOM	2571	CB	LEU	A	333	50.033	83.478	24.729	1.00	0.00
ATOM	2572	CG	LEU	A	333	50.560	83.254	26.153	1.00	0.00

Figure 1A-47

ATOM	2573	CD1	LEU	A	333	51.983	82.754	26.132	1.00	0.00
ATOM	2574	CD2	LEU	A	333	50.450	84.554	26.941	1.00	0.00
ATOM	2575	C	LEU	A	333	49.414	82.365	22.563	1.00	0.00
ATOM	2576	O	LEU	A	333	48.320	81.916	22.912	1.00	0.00
ATOM	2577	N	THR	A	334	49.688	82.692	21.300	1.00	0.00
ATOM	2578	CA	THR	A	334	48.703	82.545	20.214	1.00	0.00
ATOM	2579	CB	THR	A	334	47.935	83.868	19.957	1.00	0.00
ATOM	2580	OG1	THR	A	334	48.856	84.966	19.967	1.00	0.00
ATOM	2581	CG2	THR	A	334	46.870	84.096	21.021	1.00	0.00
ATOM	2582	C	THR	A	334	49.371	82.130	18.905	1.00	0.00
ATOM	2583	O	THR	A	334	50.539	82.431	18.681	1.00	0.00
ATOM	2584	N	ASP	A	335	48.635	81.438	18.041	1.00	0.00
ATOM	2585	CA	ASP	A	335	49.195	81.014	16.762	1.00	0.00
ATOM	2586	CB	ASP	A	335	48.287	79.979	16.082	1.00	0.00
ATOM	2587	CG	ASP	A	335	48.893	79.414	14.794	1.00	0.00
ATOM	2588	OD1	ASP	A	335	48.360	78.409	14.268	1.00	0.00
ATOM	2589	OD2	ASP	A	335	49.899	79.975	14.302	1.00	0.00
ATOM	2590	C	ASP	A	335	49.335	82.249	15.881	1.00	0.00
ATOM	2591	O	ASP	A	335	48.379	83.007	15.716	1.00	0.00
ATOM	2592	N	PRO	A	336	50.537	82.478	15.322	1.00	0.00
ATOM	2593	CD	PRO	A	336	51.782	81.751	15.614	1.00	0.00
ATOM	2594	CA	PRO	A	336	50.811	83.630	14.454	1.00	0.00
ATOM	2595	CB	PRO	A	336	52.316	83.533	14.214	1.00	0.00
ATOM	2596	CG	PRO	A	336	52.814	82.828	15.422	1.00	0.00
ATOM	2597	C	PRO	A	336	50.018	83.582	13.147	1.00	0.00
ATOM	2598	O	PRO	A	336	49.998	84.550	12.384	1.00	0.00
ATOM	2599	N	GLY	A	337	49.377	82.442	12.899	1.00	0.00
ATOM	2600	CA	GLY	A	337	48.578	82.271	11.699	1.00	0.00
ATOM	2601	C	GLY	A	337	49.354	81.732	10.513	1.00	0.00
ATOM	2602	O	GLY	A	337	50.170	80.813	10.645	1.00	0.00
ATOM	2603	N	ASN	A	338	49.091	82.315	9.347	1.00	0.00
ATOM	2604	CA	ASN	A	338	49.739	81.922	8.101	1.00	0.00
ATOM	2605	CB	ASN	A	338	48.791	82.189	6.925	1.00	0.00
ATOM	2606	CG	ASN	A	338	48.251	83.617	6.915	1.00	0.00
ATOM	2607	OD1	ASN	A	338	47.499	84.001	6.018	1.00	0.00
ATOM	2608	ND2	ASN	A	338	48.632	84.406	7.918	1.00	0.00
ATOM	2609	C	ASN	A	338	51.058	82.662	7.882	1.00	0.00
ATOM	2610	O	ASN	A	338	51.210	83.816	8.287	1.00	0.00
ATOM	2611	N	VAL	A	339	52.006	81.989	7.236	1.00	0.00
ATOM	2612	CA	VAL	A	339	53.317	82.570	6.954	1.00	0.00
ATOM	2613	CB	VAL	A	339	53.180	83.943	6.239	1.00	0.00
ATOM	2614	CG1	VAL	A	339	54.534	84.393	5.705	1.00	0.00
ATOM	2615	CG2	VAL	A	339	52.174	83.842	5.099	1.00	0.00
ATOM	2616	C	VAL	A	339	54.101	82.740	8.257	1.00	0.00
ATOM	2617	O	VAL	A	339	55.008	83.569	8.364	1.00	0.00
ATOM	2618	N	GLN	A	340	53.734	81.936	9.249	1.00	0.00
ATOM	2619	CA	GLN	A	340	54.378	81.951	10.558	1.00	0.00
ATOM	2620	CB	GLN	A	340	53.752	83.025	11.447	1.00	0.00
ATOM	2621	CG	GLN	A	340	54.463	84.369	11.415	1.00	0.00
ATOM	2622	CD	GLN	A	340	55.810	84.330	12.112	1.00	0.00
ATOM	2623	OE1	GLN	A	340	56.691	83.553	11.740	1.00	0.00
ATOM	2624	NE2	GLN	A	340	55.977	85.169	13.129	1.00	0.00
ATOM	2625	C	GLN	A	340	54.203	80.584	11.199	1.00	0.00
ATOM	2626	O	GLN	A	340	54.012	80.468	12.410	1.00	0.00
ATOM	2627	N	LYS	A	341	54.266	79.549	10.369	1.00	0.00
ATOM	2628	CA	LYS	A	341	54.118	78.181	10.837	1.00	0.00

Figure 1A-48

ATOM	2629	CB	LYS	A	341	54.473	77.205	9.709	1.00	0.00
ATOM	2630	CG	LYS	A	341	55.831	77.454	9.065	1.00	0.00
ATOM	2631	CD	LYS	A	341	56.050	76.598	7.814	1.00	0.00
ATOM	2632	CE	LYS	A	341	56.113	75.105	8.123	1.00	0.00
ATOM	2633	NZ	LYS	A	341	54.828	74.571	8.652	1.00	0.00
ATOM	2634	C	LYS	A	341	54.984	77.915	12.068	1.00	0.00
ATOM	2635	O	LYS	A	341	56.049	78.517	12.244	1.00	0.00
ATOM	2636	N	ALA	A	342	54.511	77.012	12.919	1.00	0.00
ATOM	2637	CA	ALA	A	342	55.213	76.657	14.144	1.00	0.00
ATOM	2638	CB	ALA	A	342	55.123	77.807	15.138	1.00	0.00
ATOM	2639	C	ALA	A	342	54.571	75.415	14.736	1.00	0.00
ATOM	2640	O	ALA	A	342	53.575	74.914	14.214	1.00	0.00
ATOM	2641	N	VAL	A	343	55.149	74.910	15.820	1.00	0.00
ATOM	2642	CA	VAL	A	343	54.588	73.748	16.493	1.00	0.00
ATOM	2643	CB	VAL	A	343	55.692	72.932	17.205	1.00	0.00
ATOM	2644	CG1	VAL	A	343	56.890	72.785	16.277	1.00	0.00
ATOM	2645	CG2	VAL	A	343	56.098	73.600	18.510	1.00	0.00
ATOM	2646	C	VAL	A	343	53.595	74.330	17.506	1.00	0.00
ATOM	2647	O	VAL	A	343	53.892	75.336	18.149	1.00	0.00
ATOM	2648	N	CYS	A	344	52.423	73.713	17.643	1.00	0.00
ATOM	2649	CA	CYS	A	344	51.399	74.230	18.551	1.00	0.00
ATOM	2650	C	CYS	A	344	51.011	73.405	19.771	1.00	0.00
ATOM	2651	O	CYS	A	344	51.338	72.224	19.873	1.00	0.00
ATOM	2652	CB	CYS	A	344	50.113	74.516	17.777	1.00	0.00
ATOM	2653	SG	CYS	A	344	50.081	76.047	16.799	1.00	0.00
ATOM	2654	N	HIS	A	345	50.288	74.073	20.676	1.00	0.00
ATOM	2655	CA	HIS	A	345	49.755	73.516	21.930	1.00	0.00
ATOM	2656	CB	HIS	A	345	48.490	72.686	21.645	1.00	0.00
ATOM	2657	CG	HIS	A	345	47.266	73.497	21.360	1.00	0.00
ATOM	2658	CD2	HIS	A	345	46.142	73.699	22.090	1.00	0.00
ATOM	2659	ND1	HIS	A	345	47.085	74.185	20.179	1.00	0.00
ATOM	2660	CE1	HIS	A	345	45.901	74.772	20.193	1.00	0.00
ATOM	2661	NE2	HIS	A	345	45.308	74.493	21.341	1.00	0.00
ATOM	2662	C	HIS	A	345	50.676	72.646	22.790	1.00	0.00
ATOM	2663	O	HIS	A	345	50.214	71.644	23.349	1.00	0.00
ATOM	2664	N	PRO	A	346	51.956	73.021	22.959	1.00	0.00
ATOM	2665	CD	PRO	A	346	52.967	73.268	21.923	1.00	0.00
ATOM	2666	CA	PRO	A	346	52.428	71.926	23.798	1.00	0.00
ATOM	2667	CB	PRO	A	346	52.783	70.892	22.744	1.00	0.00
ATOM	2668	CG	PRO	A	346	53.455	71.834	21.621	1.00	0.00
ATOM	2669	C	PRO	A	346	53.632	72.156	24.706	1.00	0.00
ATOM	2670	O	PRO	A	346	54.177	71.169	25.192	1.00	0.00
ATOM	2671	N	THR	A	347	54.064	73.387	24.975	1.00	0.00
ATOM	2672	CA	THR	A	347	55.298	73.478	25.745	1.00	0.00
ATOM	2673	CB	THR	A	347	56.492	73.327	24.783	1.00	0.00
ATOM	2674	OG1	THR	A	347	56.381	74.306	23.748	1.00	0.00
ATOM	2675	CG2	THR	A	347	56.521	71.940	24.145	1.00	0.00
ATOM	2676	C	THR	A	347	55.641	74.628	26.695	1.00	0.00
ATOM	2677	O	THR	A	347	55.272	75.784	26.476	1.00	0.00
ATOM	2678	N	ALA	A	348	56.383	74.273	27.748	1.00	0.00
ATOM	2679	CA	ALA	A	348	56.855	75.219	28.768	1.00	0.00
ATOM	2680	CB	ALA	A	348	56.418	74.766	30.161	1.00	0.00
ATOM	2681	C	ALA	A	348	58.376	75.238	28.668	1.00	0.00
ATOM	2682	O	ALA	A	348	59.016	74.190	28.712	1.00	0.00
ATOM	2683	N	TRP	A	349	58.964	76.419	28.534	1.00	0.00
ATOM	2684	CA	TRP	A	349	60.409	76.488	28.377	1.00	0.00

Figure 1A-49

ATOM	2685	CB	TRP	A	349	60.775	77.217	27.077	1.00	0.00
ATOM	2686	CG	TRP	A	349	60.248	76.618	25.808	1.00	0.00
ATOM	2687	CD2	TRP	A	349	61.005	76.304	24.630	1.00	0.00
ATOM	2688	CE2	TRP	A	349	60.087	75.863	23.650	1.00	0.00
ATOM	2689	CE3	TRP	A	349	62.368	76.359	24.307	1.00	0.00
ATOM	2690	CD1	TRP	A	349	58.941	76.355	25.503	1.00	0.00
ATOM	2691	NE1	TRP	A	349	58.838	75.904	24.211	1.00	0.00
ATOM	2692	CZ2	TRP	A	349	60.486	75.479	22.359	1.00	0.00
ATOM	2693	CZ3	TRP	A	349	62.770	75.981	23.024	1.00	0.00
ATOM	2694	CH2	TRP	A	349	61.826	75.546	22.063	1.00	0.00
ATOM	2695	C	TRP	A	349	61.193	77.148	29.495	1.00	0.00
ATOM	2696	O	TRP	A	349	60.789	78.170	30.052	1.00	0.00
ATOM	2697	N	ASP	A	350	62.338	76.548	29.785	1.00	0.00
ATOM	2698	CA	ASP	A	350	63.288	77.039	30.778	1.00	0.00
ATOM	2699	CB	ASP	A	350	63.484	75.992	31.887	1.00	0.00
ATOM	2700	CG	ASP	A	350	64.477	76.443	32.967	1.00	0.00
ATOM	2701	OD1	ASP	A	350	64.393	75.915	34.094	1.00	0.00
ATOM	2702	OD2	ASP	A	350	65.346	77.308	32.701	1.00	0.00
ATOM	2703	C	ASP	A	350	64.547	77.194	29.922	1.00	0.00
ATOM	2704	O	ASP	A	350	65.360	76.293	29.826	1.00	0.00
ATOM	2705	N	LEU	A	351	64.683	78.337	29.264	1.00	0.00
ATOM	2706	CA	LEU	A	351	65.820	78.556	28.375	1.00	0.00
ATOM	2707	CB	LEU	A	351	65.550	79.740	27.441	1.00	0.00
ATOM	2708	CG	LEU	A	351	64.339	79.614	26.514	1.00	0.00
ATOM	2709	CD1	LEU	A	351	63.084	80.023	27.275	1.00	0.00
ATOM	2710	CD2	LEU	A	351	64.530	80.509	25.287	1.00	0.00
ATOM	2711	C	LEU	A	351	67.144	78.772	29.067	1.00	0.00
ATOM	2712	O	LEU	A	351	68.200	78.572	28.472	1.00	0.00
ATOM	2713	N	GLY	A	352	67.089	79.174	30.326	1.00	0.00
ATOM	2714	CA	GLY	A	352	68.298	79.427	31.068	1.00	0.00
ATOM	2715	C	GLY	A	352	68.335	80.881	31.483	1.00	0.00
ATOM	2716	O	GLY	A	352	67.482	81.681	31.083	1.00	0.00
ATOM	2717	N	LYS	A	353	69.323	81.204	32.310	1.00	0.00
ATOM	2718	CA	LYS	A	353	69.537	82.553	32.814	1.00	0.00
ATOM	2719	CB	LYS	A	353	70.394	83.333	31.815	1.00	0.00
ATOM	2720	CG	LYS	A	353	70.873	84.687	32.331	1.00	0.00
ATOM	2721	CD	LYS	A	353	71.587	84.577	33.684	1.00	0.00
ATOM	2722	CE	LYS	A	353	72.034	85.957	34.184	1.00	0.00
ATOM	2723	NZ	LYS	A	353	70.896	86.924	34.288	1.00	0.00
ATOM	2724	C	LYS	A	353	68.253	83.324	33.137	1.00	0.00
ATOM	2725	O	LYS	A	353	68.073	84.470	32.702	1.00	0.00
ATOM	2726	N	GLY	A	354	67.367	82.691	33.907	1.00	0.00
ATOM	2727	CA	GLY	A	354	66.118	83.323	34.295	1.00	0.00
ATOM	2728	C	GLY	A	354	65.123	83.599	33.175	1.00	0.00
ATOM	2729	O	GLY	A	354	64.201	84.403	33.336	1.00	0.00
ATOM	2730	N	ASP	A	355	65.297	82.935	32.040	1.00	0.00
ATOM	2731	CA	ASP	A	355	64.407	83.130	30.900	1.00	0.00
ATOM	2732	CB	ASP	A	355	65.251	83.210	29.633	1.00	0.00
ATOM	2733	CG	ASP	A	355	64.448	83.595	28.408	1.00	0.00
ATOM	2734	OD1	ASP	A	355	65.083	83.938	27.391	1.00	0.00
ATOM	2735	OD2	ASP	A	355	63.200	83.554	28.446	1.00	0.00
ATOM	2736	C	ASP	A	355	63.375	81.990	30.802	1.00	0.00
ATOM	2737	O	ASP	A	355	63.708	80.853	30.460	1.00	0.00
ATOM	2738	N	PHE	A	356	62.122	82.304	31.106	1.00	0.00
ATOM	2739	CA	PHE	A	356	61.047	81.317	31.070	1.00	0.00
ATOM	2740	CB	PHE	A	356	60.394	81.211	32.451	1.00	0.00

50/396

Figure 1A-50

ATOM	2741	CG	PHE	A	356	61.376	80.983	33.560	1.00	0.00
ATOM	2742	CD1	PHE	A	356	61.920	82.058	34.260	1.00	0.00
ATOM	2743	CD2	PHE	A	356	61.809	79.690	33.871	1.00	0.00
ATOM	2744	CE1	PHE	A	356	62.889	81.850	35.260	1.00	0.00
ATOM	2745	CE2	PHE	A	356	62.774	79.471	34.863	1.00	0.00
ATOM	2746	CZ	PHE	A	356	63.317	80.551	35.559	1.00	0.00
ATOM	2747	C	PHE	A	356	60.001	81.717	30.042	1.00	0.00
ATOM	2748	O	PHE	A	356	59.652	82.888	29.944	1.00	0.00
ATOM	2749	N	ARG	A	357	59.496	80.749	29.281	1.00	0.00
ATOM	2750	CA	ARG	A	357	58.482	81.045	28.268	1.00	0.00
ATOM	2751	CB	ARG	A	357	59.128	81.387	26.923	1.00	0.00
ATOM	2752	CG	ARG	A	357	60.157	82.497	26.960	1.00	0.00
ATOM	2753	CD	ARG	A	357	60.769	82.736	25.586	1.00	0.00
ATOM	2754	NE	ARG	A	357	61.970	83.559	25.693	1.00	0.00
ATOM	2755	CZ	ARG	A	357	62.693	83.980	24.661	1.00	0.00
ATOM	2756	NH1	ARG	A	357	63.772	84.717	24.873	1.00	0.00
ATOM	2757	NH2	ARG	A	357	62.335	83.671	23.421	1.00	0.00
ATOM	2758	C	ARG	A	357	57.556	79.877	28.023	1.00	0.00
ATOM	2759	O	ARG	A	357	57.930	78.718	28.217	1.00	0.00
ATOM	2760	N	ILE	A	358	56.339	80.190	27.593	1.00	0.00
ATOM	2761	CA	ILE	A	358	55.371	79.161	27.231	1.00	0.00
ATOM	2762	CB	ILE	A	358	54.070	79.243	28.070	1.00	0.00
ATOM	2763	CG2	ILE	A	358	52.925	78.539	27.325	1.00	0.00
ATOM	2764	CG1	ILE	A	358	54.297	78.596	29.445	1.00	0.00
ATOM	2765	CD1	ILE	A	358	53.111	78.692	30.401	1.00	0.00
ATOM	2766	C	ILE	A	358	55.041	79.360	25.752	1.00	0.00
ATOM	2767	O	ILE	A	358	54.812	80.488	25.297	1.00	0.00
ATOM	2768	N	LEU	A	359	55.064	78.260	25.006	1.00	0.00
ATOM	2769	CA	LEU	A	359	54.746	78.248	23.586	1.00	0.00
ATOM	2770	CB	LEU	A	359	55.854	77.555	22.776	1.00	0.00
ATOM	2771	CG	LEU	A	359	55.514	77.070	21.350	1.00	0.00
ATOM	2772	CD1	LEU	A	359	54.708	78.110	20.590	1.00	0.00
ATOM	2773	CD2	LEU	A	359	56.798	76.756	20.604	1.00	0.00
ATOM	2774	C	LEU	A	359	53.457	77.462	23.465	1.00	0.00
ATOM	2775	O	LEU	A	359	53.421	76.267	23.764	1.00	0.00
ATOM	2776	N	MET	A	360	52.395	78.135	23.038	1.00	0.00
ATOM	2777	CA	MET	A	360	51.107	77.485	22.900	1.00	0.00
ATOM	2778	CB	MET	A	360	50.503	77.279	24.289	1.00	0.00
ATOM	2779	CG	MET	A	360	49.405	76.236	24.381	1.00	0.00
ATOM	2780	SD	MET	A	360	48.676	76.171	26.048	1.00	0.00
ATOM	2781	CE	MET	A	360	46.973	76.544	25.721	1.00	0.00
ATOM	2782	C	MET	A	360	50.178	78.348	22.047	1.00	0.00
ATOM	2783	O	MET	A	360	50.032	79.550	22.287	1.00	0.00
ATOM	2784	N	CYS	A	361	49.554	77.736	21.046	1.00	0.00
ATOM	2785	CA	CYS	A	361	48.624	78.464	20.184	1.00	0.00
ATOM	2786	C	CYS	A	361	47.275	78.341	20.872	1.00	0.00
ATOM	2787	O	CYS	A	361	46.424	77.548	20.478	1.00	0.00
ATOM	2788	CB	CYS	A	361	48.600	77.839	18.786	1.00	0.00
ATOM	2789	SG	CYS	A	361	50.289	77.522	18.178	1.00	0.00
ATOM	2790	N	THR	A	362	47.109	79.145	21.918	1.00	0.00
ATOM	2791	CA	THR	A	362	45.910	79.151	22.742	1.00	0.00
ATOM	2792	CB	THR	A	362	46.082	80.138	23.915	1.00	0.00
ATOM	2793	OG1	THR	A	362	47.315	79.865	24.593	1.00	0.00
ATOM	2794	CG2	THR	A	362	44.939	80.000	24.905	1.00	0.00
ATOM	2795	C	THR	A	362	44.593	79.465	22.034	1.00	0.00
ATOM	2796	O	THR	A	362	44.493	80.422	21.271	1.00	0.00

Figure 1A-51

ATOM	2797	N	LYS	A	363	43.589	78.637	22.309	1.00	0.00
ATOM	2798	CA	LYS	A	363	42.244	78.796	21.765	1.00	0.00
ATOM	2799	CB	LYS	A	363	41.783	77.513	21.076	1.00	0.00
ATOM	2800	CG	LYS	A	363	42.663	77.048	19.928	1.00	0.00
ATOM	2801	CD	LYS	A	363	42.181	75.691	19.413	1.00	0.00
ATOM	2802	CE	LYS	A	363	43.077	75.139	18.310	1.00	0.00
ATOM	2803	NZ	LYS	A	363	42.570	73.831	17.800	1.00	0.00
ATOM	2804	C	LYS	A	363	41.332	79.077	22.959	1.00	0.00
ATOM	2805	O	LYS	A	363	41.629	78.656	24.082	1.00	0.00
ATOM	2806	N	VAL	A	364	40.226	79.778	22.726	1.00	0.00
ATOM	2807	CA	VAL	A	364	39.301	80.107	23.804	1.00	0.00
ATOM	2808	CB	VAL	A	364	38.432	81.322	23.432	1.00	0.00
ATOM	2809	CG1	VAL	A	364	37.542	81.715	24.609	1.00	0.00
ATOM	2810	CG2	VAL	A	364	39.328	82.480	23.040	1.00	0.00
ATOM	2811	C	VAL	A	364	38.393	78.932	24.160	1.00	0.00
ATOM	2812	O	VAL	A	364	37.185	78.971	23.926	1.00	0.00
ATOM	2813	N	THR	A	365	38.985	77.893	24.738	1.00	0.00
ATOM	2814	CA	THR	A	365	38.248	76.701	25.129	1.00	0.00
ATOM	2815	CB	THR	A	365	38.658	75.511	24.265	1.00	0.00
ATOM	2816	OG1	THR	A	365	38.341	75.799	22.898	1.00	0.00
ATOM	2817	CG2	THR	A	365	37.920	74.243	24.697	1.00	0.00
ATOM	2818	C	THR	A	365	38.522	76.360	26.583	1.00	0.00
ATOM	2819	O	THR	A	365	39.474	76.865	27.176	1.00	0.00
ATOM	2820	N	MET	A	366	37.680	75.513	27.163	1.00	0.00
ATOM	2821	CA	MET	A	366	37.880	75.105	28.541	1.00	0.00
ATOM	2822	CB	MET	A	366	36.714	74.243	29.030	1.00	0.00
ATOM	2823	CG	MET	A	366	36.720	74.005	30.537	1.00	0.00
ATOM	2824	SD	MET	A	366	35.419	72.887	31.117	1.00	0.00
ATOM	2825	CE	MET	A	366	36.296	71.302	30.985	1.00	0.00
ATOM	2826	C	MET	A	366	39.170	74.294	28.566	1.00	0.00
ATOM	2827	O	MET	A	366	39.990	74.433	29.473	1.00	0.00
ATOM	2828	N	ASP	A	367	39.357	73.463	27.548	1.00	0.00
ATOM	2829	CA	ASP	A	367	40.548	72.635	27.467	1.00	0.00
ATOM	2830	CB	ASP	A	367	40.503	71.761	26.213	1.00	0.00
ATOM	2831	CG	ASP	A	367	39.584	70.552	26.374	1.00	0.00
ATOM	2832	OD1	ASP	A	367	38.834	70.487	27.378	1.00	0.00
ATOM	2833	OD2	ASP	A	367	39.609	69.668	25.490	1.00	0.00
ATOM	2834	C	ASP	A	367	41.854	73.421	27.501	1.00	0.00
ATOM	2835	O	ASP	A	367	42.797	73.018	28.178	1.00	0.00
ATOM	2836	N	ASP	A	368	41.920	74.541	26.786	1.00	0.00
ATOM	2837	CA	ASP	A	368	43.146	75.333	26.766	1.00	0.00
ATOM	2838	CB	ASP	A	368	43.196	76.204	25.513	1.00	0.00
ATOM	2839	CG	ASP	A	368	43.573	75.409	24.297	1.00	0.00
ATOM	2840	OD1	ASP	A	368	43.065	74.278	24.167	1.00	0.00
ATOM	2841	OD2	ASP	A	368	44.369	75.900	23.471	1.00	0.00
ATOM	2842	C	ASP	A	368	43.326	76.176	28.009	1.00	0.00
ATOM	2843	O	ASP	A	368	44.420	76.664	28.287	1.00	0.00
ATOM	2844	N	PHE	A	369	42.245	76.346	28.756	1.00	0.00
ATOM	2845	CA	PHE	A	369	42.292	77.101	29.996	1.00	0.00
ATOM	2846	CB	PHE	A	369	40.862	77.506	30.392	1.00	0.00
ATOM	2847	CG	PHE	A	369	40.704	77.923	31.836	1.00	0.00
ATOM	2848	CD1	PHE	A	369	40.382	76.983	32.817	1.00	0.00
ATOM	2849	CD2	PHE	A	369	40.820	79.258	32.205	1.00	0.00
ATOM	2850	CE1	PHE	A	369	40.174	77.364	34.139	1.00	0.00
ATOM	2851	CE2	PHE	A	369	40.612	79.655	33.530	1.00	0.00
ATOM	2852	CZ	PHE	A	369	40.286	78.701	34.499	1.00	0.00

Figure 1A-52

ATOM	2853	C	PHE	A	369	42.956	76.212	31.064	1.00	0.00
ATOM	2854	O	PHE	A	369	43.662	76.702	31.947	1.00	0.00
ATOM	2855	N	LEU	A	370	42.739	74.902	30.956	1.00	0.00
ATOM	2856	CA	LEU	A	370	43.307	73.936	31.894	1.00	0.00
ATOM	2857	CB	LEU	A	370	42.488	72.644	31.890	1.00	0.00
ATOM	2858	CG	LEU	A	370	41.008	72.821	32.220	1.00	0.00
ATOM	2859	CD1	LEU	A	370	40.267	71.514	31.987	1.00	0.00
ATOM	2860	CD2	LEU	A	370	40.863	73.299	33.662	1.00	0.00
ATOM	2861	C	LEU	A	370	44.744	73.626	31.508	1.00	0.00
ATOM	2862	O	LEU	A	370	45.597	73.421	32.374	1.00	0.00
ATOM	2863	N	THR	A	371	45.011	73.587	30.204	1.00	0.00
ATOM	2864	CA	THR	A	371	46.362	73.312	29.727	1.00	0.00
ATOM	2865	CB	THR	A	371	46.393	73.131	28.199	1.00	0.00
ATOM	2866	OG1	THR	A	371	45.805	71.872	27.863	1.00	0.00
ATOM	2867	CG2	THR	A	371	47.811	73.149	27.685	1.00	0.00
ATOM	2868	C	THR	A	371	47.294	74.449	30.132	1.00	0.00
ATOM	2869	O	THR	A	371	48.468	74.228	30.463	1.00	0.00
ATOM	2870	N	ALA	A	372	46.759	75.664	30.115	1.00	0.00
ATOM	2871	CA	ALA	A	372	47.526	76.837	30.502	1.00	0.00
ATOM	2872	CB	ALA	A	372	46.689	78.095	30.320	1.00	0.00
ATOM	2873	C	ALA	A	372	47.949	76.699	31.968	1.00	0.00
ATOM	2874	O	ALA	A	372	49.079	77.032	32.323	1.00	0.00
ATOM	2875	N	HIS	A	373	47.037	76.234	32.817	1.00	0.00
ATOM	2876	CA	HIS	A	373	47.351	76.055	34.227	1.00	0.00
ATOM	2877	CB	HIS	A	373	46.095	75.692	35.023	1.00	0.00
ATOM	2878	CG	HIS	A	373	45.195	76.856	35.292	1.00	0.00
ATOM	2879	CD2	HIS	A	373	45.011	77.598	36.410	1.00	0.00
ATOM	2880	ND1	HIS	A	373	44.354	77.387	34.338	1.00	0.00
ATOM	2881	CE1	HIS	A	373	43.690	78.405	34.857	1.00	0.00
ATOM	2882	NE2	HIS	A	373	44.070	78.554	36.113	1.00	0.00
ATOM	2883	C	HIS	A	373	48.394	74.946	34.361	1.00	0.00
ATOM	2884	O	HIS	A	373	49.397	75.093	35.070	1.00	0.00
ATOM	2885	N	HIS	A	374	48.158	73.835	33.666	1.00	0.00
ATOM	2886	CA	HIS	A	374	49.097	72.730	33.697	1.00	0.00
ATOM	2887	CB	HIS	A	374	48.636	71.621	32.744	1.00	0.00
ATOM	2888	CG	HIS	A	374	49.681	70.585	32.464	1.00	0.00
ATOM	2889	CD2	HIS	A	374	50.918	70.689	31.919	1.00	0.00
ATOM	2890	ND1	HIS	A	374	49.487	69.244	32.719	1.00	0.00
ATOM	2891	CE1	HIS	A	374	50.560	68.566	32.336	1.00	0.00
ATOM	2892	NE2	HIS	A	374	51.446	69.420	31.848	1.00	0.00
ATOM	2893	C	HIS	A	374	50.474	73.243	33.285	1.00	0.00
ATOM	2894	O	HIS	A	374	51.451	73.099	34.027	1.00	0.00
ATOM	2895	N	GLU	A	375	50.547	73.850	32.097	1.00	0.00
ATOM	2896	CA	GLU	A	375	51.810	74.362	31.589	1.00	0.00
ATOM	2897	CB	GLU	A	375	51.652	74.846	30.149	1.00	0.00
ATOM	2898	CG	GLU	A	375	51.364	73.721	29.140	1.00	0.00
ATOM	2899	CD	GLU	A	375	52.427	72.627	29.133	1.00	0.00
ATOM	2900	OE1	GLU	A	375	53.632	72.960	29.123	1.00	0.00
ATOM	2901	OE2	GLU	A	375	52.062	71.431	29.123	1.00	0.00
ATOM	2902	C	GLU	A	375	52.411	75.460	32.464	1.00	0.00
ATOM	2903	O	GLU	A	375	53.625	75.506	32.659	1.00	0.00
ATOM	2904	N	MET	A	376	51.594	76.351	33.005	1.00	0.00
ATOM	2905	CA	MET	A	376	52.189	77.360	33.858	1.00	0.00
ATOM	2906	CB	MET	A	376	51.191	78.464	34.201	1.00	0.00
ATOM	2907	CG	MET	A	376	51.843	79.676	34.870	1.00	0.00
ATOM	2908	SD	MET	A	376	50.699	81.052	35.138	1.00	0.00

Figure 1A-53

ATOM	2909	CE	MET	A	376	50.785	81.788	33.485	1.00	0.00
ATOM	2910	C	MET	A	376	52.677	76.678	35.138	1.00	0.00
ATOM	2911	O	MET	A	376	53.458	77.251	35.886	1.00	0.00
ATOM	2912	N	GLY	A	377	52.206	75.455	35.388	1.00	0.00
ATOM	2913	CA	GLY	A	377	52.622	74.721	36.571	1.00	0.00
ATOM	2914	C	GLY	A	377	54.082	74.354	36.422	1.00	0.00
ATOM	2915	O	GLY	A	377	54.854	74.388	37.383	1.00	0.00
ATOM	2916	N	HIS	A	378	54.459	74.000	35.199	1.00	0.00
ATOM	2917	CA	HIS	A	378	55.832	73.649	34.877	1.00	0.00
ATOM	2918	CB	HIS	A	378	55.944	73.195	33.434	1.00	0.00
ATOM	2919	CG	HIS	A	378	55.380	71.842	33.173	1.00	0.00
ATOM	2920	CD2	HIS	A	378	54.483	71.415	32.255	1.00	0.00
ATOM	2921	ND1	HIS	A	378	55.833	70.714	33.822	1.00	0.00
ATOM	2922	CE1	HIS	A	378	55.246	69.649	33.309	1.00	0.00
ATOM	2923	NE2	HIS	A	378	54.424	70.048	32.356	1.00	0.00
ATOM	2924	C	HIS	A	378	56.788	74.829	35.038	1.00	0.00
ATOM	2925	O	HIS	A	378	57.927	74.669	35.485	1.00	0.00
ATOM	2926	N	ILE	A	379	56.340	76.001	34.603	1.00	0.00
ATOM	2927	CA	ILE	A	379	57.162	77.197	34.686	1.00	0.00
ATOM	2928	CB	ILE	A	379	56.420	78.411	34.080	1.00	0.00
ATOM	2929	CG2	ILE	A	379	57.274	79.674	34.241	1.00	0.00
ATOM	2930	CG1	ILE	A	379	56.114	78.150	32.601	1.00	0.00
ATOM	2931	CD1	ILE	A	379	57.358	78.046	31.717	1.00	0.00
ATOM	2932	C	ILE	A	379	57.476	77.475	36.157	1.00	0.00
ATOM	2933	O	ILE	A	379	58.629	77.698	36.552	1.00	0.00
ATOM	2934	N	GLN	A	380	56.420	77.431	36.953	1.00	0.00
ATOM	2935	CA	GLN	A	380	56.492	77.668	38.377	1.00	0.00
ATOM	2936	CB	GLN	A	380	55.132	77.351	38.985	1.00	0.00
ATOM	2937	CG	GLN	A	380	54.863	78.079	40.248	1.00	0.00
ATOM	2938	CD	GLN	A	380	54.750	79.558	40.014	1.00	0.00
ATOM	2939	OE1	GLN	A	380	55.321	80.345	40.750	1.00	0.00
ATOM	2940	NE2	GLN	A	380	54.001	79.948	38.987	1.00	0.00
ATOM	2941	C	GLN	A	380	57.565	76.776	38.996	1.00	0.00
ATOM	2942	O	GLN	A	380	58.387	77.222	39.805	1.00	0.00
ATOM	2943	N	TYR	A	381	57.550	75.513	38.596	1.00	0.00
ATOM	2944	CA	TYR	A	381	58.491	74.538	39.097	1.00	0.00
ATOM	2945	CB	TYR	A	381	58.097	73.143	38.590	1.00	0.00
ATOM	2946	CG	TYR	A	381	58.705	71.955	39.318	1.00	0.00
ATOM	2947	CD1	TYR	A	381	58.187	70.666	39.119	1.00	0.00
ATOM	2948	CE1	TYR	A	381	58.721	69.551	39.779	1.00	0.00
ATOM	2949	CD2	TYR	A	381	59.782	72.105	40.198	1.00	0.00
ATOM	2950	CE2	TYR	A	381	60.329	70.996	40.866	1.00	0.00
ATOM	2951	CZ	TYR	A	381	59.792	69.722	40.648	1.00	0.00
ATOM	2952	OH	TYR	A	381	60.340	68.618	41.246	1.00	0.00
ATOM	2953	C	TYR	A	381	59.879	74.927	38.618	1.00	0.00
ATOM	2954	O	TYR	A	381	60.847	74.810	39.362	1.00	0.00
ATOM	2955	N	ASP	A	382	59.980	75.400	37.383	1.00	0.00
ATOM	2956	CA	ASP	A	382	61.266	75.817	36.834	1.00	0.00
ATOM	2957	CB	ASP	A	382	61.122	76.179	35.362	1.00	0.00
ATOM	2958	CG	ASP	A	382	60.775	74.991	34.495	1.00	0.00
ATOM	2959	OD1	ASP	A	382	61.370	73.906	34.690	1.00	0.00
ATOM	2960	OD2	ASP	A	382	59.920	75.159	33.599	1.00	0.00
ATOM	2961	C	ASP	A	382	61.825	77.040	37.574	1.00	0.00
ATOM	2962	O	ASP	A	382	63.033	77.146	37.819	1.00	0.00
ATOM	2963	N	MET	A	383	60.940	77.970	37.910	1.00	0.00
ATOM	2964	CA	MET	A	383	61.342	79.175	38.610	1.00	0.00

Figure 1A-54

ATOM	2965	CB	MET	A	383	60.189	80.178	38.624	1.00	0.00
ATOM	2966	CG	MET	A	383	59.866	80.753	37.245	1.00	0.00
ATOM	2967	SD	MET	A	383	58.323	81.665	37.251	1.00	0.00
ATOM	2968	CE	MET	A	383	58.618	82.863	38.530	1.00	0.00
ATOM	2969	C	MET	A	383	61.779	78.868	40.034	1.00	0.00
ATOM	2970	O	MET	A	383	62.776	79.409	40.513	1.00	0.00
ATOM	2971	N	ALA	A	384	61.042	77.986	40.698	1.00	0.00
ATOM	2972	CA	ALA	A	384	61.340	77.621	42.074	1.00	0.00
ATOM	2973	CB	ALA	A	384	60.277	76.635	42.593	1.00	0.00
ATOM	2974	C	ALA	A	384	62.743	77.049	42.278	1.00	0.00
ATOM	2975	O	ALA	A	384	63.353	77.264	43.320	1.00	0.00
ATOM	2976	N	TYR	A	385	63.270	76.326	41.298	1.00	0.00
ATOM	2977	CA	TYR	A	385	64.605	75.758	41.457	1.00	0.00
ATOM	2978	CB	TYR	A	385	64.563	74.235	41.227	1.00	0.00
ATOM	2979	CG	TYR	A	385	64.076	73.757	39.864	1.00	0.00
ATOM	2980	CD1	TYR	A	385	63.212	72.665	39.773	1.00	0.00
ATOM	2981	CE1	TYR	A	385	62.848	72.109	38.537	1.00	0.00
ATOM	2982	CD2	TYR	A	385	64.563	74.304	38.670	1.00	0.00
ATOM	2983	CE2	TYR	A	385	64.202	73.748	37.414	1.00	0.00
ATOM	2984	CZ	TYR	A	385	63.345	72.642	37.370	1.00	0.00
ATOM	2985	OH	TYR	A	385	63.019	72.026	36.176	1.00	0.00
ATOM	2986	C	TYR	A	385	65.682	76.391	40.574	1.00	0.00
ATOM	2987	O	TYR	A	385	66.740	75.804	40.361	1.00	0.00
ATOM	2988	N	ALA	A	386	65.412	77.588	40.063	1.00	0.00
ATOM	2989	CA	ALA	A	386	66.370	78.270	39.202	1.00	0.00
ATOM	2990	CB	ALA	A	386	65.763	79.561	38.682	1.00	0.00
ATOM	2991	C	ALA	A	386	67.711	78.559	39.888	1.00	0.00
ATOM	2992	O	ALA	A	386	68.745	78.625	39.221	1.00	0.00
ATOM	2993	N	ALA	A	387	67.706	78.707	41.213	1.00	0.00
ATOM	2994	CA	ALA	A	387	68.939	79.005	41.950	1.00	0.00
ATOM	2995	CB	ALA	A	387	68.607	79.592	43.312	1.00	0.00
ATOM	2996	C	ALA	A	387	69.847	77.800	42.124	1.00	0.00
ATOM	2997	O	ALA	A	387	71.025	77.942	42.468	1.00	0.00
ATOM	2998	N	GLN	A	388	69.305	76.609	41.912	1.00	0.00
ATOM	2999	CA	GLN	A	388	70.105	75.393	42.045	1.00	0.00
ATOM	3000	CB	GLN	A	388	69.199	74.163	41.914	1.00	0.00
ATOM	3001	CG	GLN	A	388	68.173	73.995	43.029	1.00	0.00
ATOM	3002	CD	GLN	A	388	68.798	73.571	44.347	1.00	0.00
ATOM	3003	OE1	GLN	A	388	69.818	72.887	44.365	1.00	0.00
ATOM	3004	NE2	GLN	A	388	68.169	73.951	45.458	1.00	0.00
ATOM	3005	C	GLN	A	388	71.145	75.365	40.929	1.00	0.00
ATOM	3006	O	GLN	A	388	70.984	76.035	39.915	1.00	0.00
ATOM	3007	N	PRO	A	389	72.251	74.631	41.112	1.00	0.00
ATOM	3008	CD	PRO	A	389	72.838	74.007	42.307	1.00	0.00
ATOM	3009	CA	PRO	A	389	73.198	74.627	39.994	1.00	0.00
ATOM	3010	CB	PRO	A	389	74.397	73.852	40.540	1.00	0.00
ATOM	3011	CG	PRO	A	389	73.828	73.062	41.695	1.00	0.00
ATOM	3012	C	PRO	A	389	72.556	73.937	38.771	1.00	0.00
ATOM	3013	O	PRO	A	389	71.662	73.101	38.913	1.00	0.00
ATOM	3014	N	PHE	A	390	73.029	74.309	37.587	1.00	0.00
ATOM	3015	CA	PHE	A	390	72.541	73.798	36.316	1.00	0.00
ATOM	3016	CB	PHE	A	390	73.618	73.989	35.251	1.00	0.00
ATOM	3017	CG	PHE	A	390	73.158	73.656	33.873	1.00	0.00
ATOM	3018	CD1	PHE	A	390	72.525	74.612	33.093	1.00	0.00
ATOM	3019	CD2	PHE	A	390	73.318	72.371	33.369	1.00	0.00
ATOM	3020	CE1	PHE	A	390	72.051	74.291	31.818	1.00	0.00

Figure 1A-55

ATOM	3021	CE2	PHE	A	390	72.850	72.037	32.103	1.00	0.00
ATOM	3022	CZ	PHE	A	390	72.214	72.999	31.325	1.00	0.00
ATOM	3023	C	PHE	A	390	72.076	72.338	36.279	1.00	0.00
ATOM	3024	O	PHE	A	390	70.940	72.045	35.891	1.00	0.00
ATOM	3025	N	LEU	A	391	72.971	71.431	36.654	1.00	0.00
ATOM	3026	CA	LEU	A	391	72.685	69.999	36.642	1.00	0.00
ATOM	3027	CB	LEU	A	391	73.972	69.205	36.868	1.00	0.00
ATOM	3028	CG	LEU	A	391	74.922	69.184	35.673	1.00	0.00
ATOM	3029	CD1	LEU	A	391	76.307	68.724	36.104	1.00	0.00
ATOM	3030	CD2	LEU	A	391	74.344	68.283	34.585	1.00	0.00
ATOM	3031	C	LEU	A	391	71.627	69.534	37.634	1.00	0.00
ATOM	3032	O	LEU	A	391	71.124	68.407	37.513	1.00	0.00
ATOM	3033	N	LEU	A	392	71.275	70.380	38.601	1.00	0.00
ATOM	3034	CA	LEU	A	392	70.264	70.000	39.584	1.00	0.00
ATOM	3035	CB	LEU	A	392	70.729	70.374	40.996	1.00	0.00
ATOM	3036	CG	LEU	A	392	71.575	69.352	41.755	1.00	0.00
ATOM	3037	CD1	LEU	A	392	72.285	68.414	40.803	1.00	0.00
ATOM	3038	CD2	LEU	A	392	72.561	70.096	42.658	1.00	0.00
ATOM	3039	C	LEU	A	392	68.919	70.650	39.305	1.00	0.00
ATOM	3040	O	LEU	A	392	67.984	70.532	40.100	1.00	0.00
ATOM	3041	N	ARG	A	393	68.821	71.349	38.182	1.00	0.00
ATOM	3042	CA	ARG	A	393	67.569	71.997	37.835	1.00	0.00
ATOM	3043	CB	ARG	A	393	67.819	73.267	37.025	1.00	0.00
ATOM	3044	CG	ARG	A	393	68.572	74.358	37.738	1.00	0.00
ATOM	3045	CD	ARG	A	393	68.587	75.593	36.865	1.00	0.00
ATOM	3046	NE	ARG	A	393	69.776	76.398	37.094	1.00	0.00
ATOM	3047	CZ	ARG	A	393	70.291	77.229	36.197	1.00	0.00
ATOM	3048	NH1	ARG	A	393	69.721	77.364	35.005	1.00	0.00
ATOM	3049	NH2	ARG	A	393	71.382	77.924	36.492	1.00	0.00
ATOM	3050	C	ARG	A	393	66.667	71.060	37.028	1.00	0.00
ATOM	3051	O	ARG	A	393	66.710	71.043	35.796	1.00	0.00
ATOM	3052	N	ASN	A	394	65.864	70.281	37.739	1.00	0.00
ATOM	3053	CA	ASN	A	394	64.927	69.357	37.125	1.00	0.00
ATOM	3054	CB	ASN	A	394	65.674	68.225	36.431	1.00	0.00
ATOM	3055	CG	ASN	A	394	64.909	67.677	35.227	1.00	0.00
ATOM	3056	OD1	ASN	A	394	65.498	67.073	34.332	1.00	0.00
ATOM	3057	ND2	ASN	A	394	63.592	67.878	35.209	1.00	0.00
ATOM	3058	C	ASN	A	394	64.036	68.817	38.236	1.00	0.00
ATOM	3059	O	ASN	A	394	64.245	69.148	39.407	1.00	0.00
ATOM	3060	N	GLY	A	395	63.028	68.023	37.878	1.00	0.00
ATOM	3061	CA	GLY	A	395	62.154	67.462	38.896	1.00	0.00
ATOM	3062	C	GLY	A	395	62.920	66.461	39.754	1.00	0.00
ATOM	3063	O	GLY	A	395	63.915	65.909	39.287	1.00	0.00
ATOM	3064	N	ALA	A	396	62.467	66.225	40.990	1.00	0.00
ATOM	3065	CA	ALA	A	396	63.132	65.271	41.900	1.00	0.00
ATOM	3066	CB	ALA	A	396	62.255	64.998	43.119	1.00	0.00
ATOM	3067	C	ALA	A	396	63.453	63.983	41.150	1.00	0.00
ATOM	3068	O	ALA	A	396	64.555	63.438	41.281	1.00	0.00
ATOM	3069	N	ASN	A	397	62.484	63.466	40.394	1.00	0.00
ATOM	3070	CA	ASN	A	397	62.734	62.313	39.531	1.00	0.00
ATOM	3071	CB	ASN	A	397	62.616	60.958	40.282	1.00	0.00
ATOM	3072	CG	ASN	A	397	61.205	60.577	40.661	1.00	0.00
ATOM	3073	OD1	ASN	A	397	60.999	59.926	41.702	1.00	0.00
ATOM	3074	ND2	ASN	A	397	60.231	60.935	39.830	1.00	0.00
ATOM	3075	C	ASN	A	397	61.845	62.404	38.280	1.00	0.00
ATOM	3076	O	ASN	A	397	61.030	63.313	38.172	1.00	0.00

56/396

Figure 1A-56

ATOM	3077	N	GLU	A	398	62.022	61.477	37.342	1.00	0.00
ATOM	3078	CA	GLU	A	398	61.291	61.492	36.074	1.00	0.00
ATOM	3079	CB	GLU	A	398	61.547	60.190	35.295	1.00	0.00
ATOM	3080	CG	GLU	A	398	61.099	58.902	35.990	1.00	0.00
ATOM	3081	CD	GLU	A	398	61.341	57.678	35.128	1.00	0.00
ATOM	3082	OE1	GLU	A	398	62.268	57.700	34.292	1.00	0.00
ATOM	3083	OE2	GLU	A	398	60.618	56.676	35.283	1.00	0.00
ATOM	3084	C	GLU	A	398	59.801	61.760	36.163	1.00	0.00
ATOM	3085	O	GLU	A	398	59.214	62.356	35.259	1.00	0.00
ATOM	3086	N	GLY	A	399	59.193	61.395	37.280	1.00	0.00
ATOM	3087	CA	GLY	A	399	57.766	61.589	37.422	1.00	0.00
ATOM	3088	C	GLY	A	399	57.213	62.775	38.171	1.00	0.00
ATOM	3089	O	GLY	A	399	56.000	62.857	38.282	1.00	0.00
ATOM	3090	N	PHE	A	400	58.048	63.690	38.671	1.00	0.00
ATOM	3091	CA	PHE	A	400	57.546	64.870	39.433	1.00	0.00
ATOM	3092	CB	PHE	A	400	58.679	65.448	40.321	1.00	0.00
ATOM	3093	CG	PHE	A	400	58.796	64.809	41.705	1.00	0.00
ATOM	3094	CD1	PHE	A	400	58.923	63.429	41.855	1.00	0.00
ATOM	3095	CD2	PHE	A	400	58.811	65.609	42.854	1.00	0.00
ATOM	3096	CE1	PHE	A	400	59.065	62.849	43.134	1.00	0.00
ATOM	3097	CE2	PHE	A	400	58.955	65.041	44.141	1.00	0.00
ATOM	3098	CZ	PHE	A	400	59.081	63.662	44.278	1.00	0.00
ATOM	3099	C	PHE	A	400	56.934	66.060	38.629	1.00	0.00
ATOM	3100	O	PHE	A	400	55.889	66.590	38.998	1.00	0.00
ATOM	3101	N	HIS	A	401	57.604	66.496	37.561	1.00	0.00
ATOM	3102	CA	HIS	A	401	57.149	67.642	36.756	1.00	0.00
ATOM	3103	CB	HIS	A	401	58.115	67.865	35.559	1.00	0.00
ATOM	3104	CG	HIS	A	401	58.830	69.184	35.593	1.00	0.00
ATOM	3105	CD2	HIS	A	401	60.135	69.487	35.796	1.00	0.00
ATOM	3106	ND1	HIS	A	401	58.176	70.391	35.451	1.00	0.00
ATOM	3107	CE1	HIS	A	401	59.044	71.379	35.568	1.00	0.00
ATOM	3108	NE2	HIS	A	401	60.241	70.858	35.778	1.00	0.00
ATOM	3109	C	HIS	A	401	55.706	67.491	36.255	1.00	0.00
ATOM	3110	O	HIS	A	401	54.878	68.390	36.455	1.00	0.00
ATOM	3111	N	GLU	A	402	55.392	66.363	35.621	1.00	0.00
ATOM	3112	CA	GLU	A	402	54.027	66.167	35.143	1.00	0.00
ATOM	3113	CB	GLU	A	402	53.956	64.976	34.170	1.00	0.00
ATOM	3114	CG	GLU	A	402	54.650	65.278	32.840	1.00	0.00
ATOM	3115	CD	GLU	A	402	54.000	66.446	32.102	1.00	0.00
ATOM	3116	OE1	GLU	A	402	54.702	67.154	31.347	1.00	0.00
ATOM	3117	OE2	GLU	A	402	52.777	66.654	32.261	1.00	0.00
ATOM	3118	C	GLU	A	402	53.044	65.990	36.296	1.00	0.00
ATOM	3119	O	GLU	A	402	51.873	66.345	36.174	1.00	0.00
ATOM	3120	N	ALA	A	403	53.492	65.443	37.422	1.00	0.00
ATOM	3121	CA	ALA	A	403	52.569	65.305	38.551	1.00	0.00
ATOM	3122	CB	ALA	A	403	53.229	64.549	39.722	1.00	0.00
ATOM	3123	C	ALA	A	403	52.197	66.717	38.985	1.00	0.00
ATOM	3124	O	ALA	A	403	51.036	67.002	39.294	1.00	0.00
ATOM	3125	N	VAL	A	404	53.191	67.604	39.009	1.00	0.00
ATOM	3126	CA	VAL	A	404	52.955	68.995	39.397	1.00	0.00
ATOM	3127	CB	VAL	A	404	54.298	69.766	39.504	1.00	0.00
ATOM	3128	CG1	VAL	A	404	54.043	71.284	39.601	1.00	0.00
ATOM	3129	CG2	VAL	A	404	55.072	69.264	40.745	1.00	0.00
ATOM	3130	C	VAL	A	404	52.025	69.688	38.387	1.00	0.00
ATOM	3131	O	VAL	A	404	51.114	70.447	38.759	1.00	0.00
ATOM	3132	N	GLY	A	405	52.256	69.414	37.107	1.00	0.00

57/396

Figure 1A-57

ATOM	3133	CA	GLY	A	405	51.415	69.999	36.081	1.00	0.00
ATOM	3134	C	GLY	A	405	49.969	69.533	36.156	1.00	0.00
ATOM	3135	O	GLY	A	405	49.056	70.362	36.089	1.00	0.00
ATOM	3136	N	GLU	A	406	49.762	68.220	36.296	1.00	0.00
ATOM	3137	CA	GLU	A	406	48.418	67.629	36.375	1.00	0.00
ATOM	3138	CB	GLU	A	406	48.510	66.103	36.464	1.00	0.00
ATOM	3139	CG	GLU	A	406	49.040	65.410	35.223	1.00	0.00
ATOM	3140	CD	GLU	A	406	48.066	65.445	34.055	1.00	0.00
ATOM	3141	OE1	GLU	A	406	46.856	65.666	34.280	1.00	0.00
ATOM	3142	OE2	GLU	A	406	48.514	65.233	32.907	1.00	0.00
ATOM	3143	C	GLU	A	406	47.619	68.137	37.570	1.00	0.00
ATOM	3144	O	GLU	A	406	46.391	68.265	37.524	1.00	0.00
ATOM	3145	N	ILE	A	407	48.326	68.404	38.655	1.00	0.00
ATOM	3146	CA	ILE	A	407	47.712	68.903	39.874	1.00	0.00
ATOM	3147	CB	ILE	A	407	48.810	69.101	40.958	1.00	0.00
ATOM	3148	CG2	ILE	A	407	48.349	70.037	42.037	1.00	0.00
ATOM	3149	CG1	ILE	A	407	49.231	67.735	41.496	1.00	0.00
ATOM	3150	CD1	ILE	A	407	48.079	66.846	41.813	1.00	0.00
ATOM	3151	C	ILE	A	407	46.986	70.226	39.638	1.00	0.00
ATOM	3152	O	ILE	A	407	45.906	70.455	40.164	1.00	0.00
ATOM	3153	N	MET	A	408	47.586	71.102	38.845	1.00	0.00
ATOM	3154	CA	MET	A	408	46.989	72.397	38.591	1.00	0.00
ATOM	3155	CB	MET	A	408	47.995	73.281	37.846	1.00	0.00
ATOM	3156	CG	MET	A	408	49.335	73.392	38.552	1.00	0.00
ATOM	3157	SD	MET	A	408	49.145	73.527	40.349	1.00	0.00
ATOM	3158	CE	MET	A	408	50.781	73.062	40.908	1.00	0.00
ATOM	3159	C	MET	A	408	45.649	72.330	37.847	1.00	0.00
ATOM	3160	O	MET	A	408	44.735	73.082	38.167	1.00	0.00
ATOM	3161	N	SER	A	409	45.522	71.426	36.879	1.00	0.00
ATOM	3162	CA	SER	A	409	44.273	71.298	36.128	1.00	0.00
ATOM	3163	CB	SER	A	409	44.428	70.333	34.950	1.00	0.00
ATOM	3164	OG	SER	A	409	45.528	70.685	34.145	1.00	0.00
ATOM	3165	C	SER	A	409	43.177	70.766	37.031	1.00	0.00
ATOM	3166	O	SER	A	409	42.007	71.147	36.899	1.00	0.00
ATOM	3167	N	LEU	A	410	43.556	69.871	37.939	1.00	0.00
ATOM	3168	CA	LEU	A	410	42.602	69.283	38.864	1.00	0.00
ATOM	3169	CB	LEU	A	410	43.334	68.388	39.863	1.00	0.00
ATOM	3170	CG	LEU	A	410	42.852	66.939	40.004	1.00	0.00
ATOM	3171	CD1	LEU	A	410	42.720	66.275	38.631	1.00	0.00
ATOM	3172	CD2	LEU	A	410	43.828	66.181	40.891	1.00	0.00
ATOM	3173	C	LEU	A	410	41.837	70.393	39.586	1.00	0.00
ATOM	3174	O	LEU	A	410	40.615	70.456	39.503	1.00	0.00
ATOM	3175	N	SER	A	411	42.548	71.287	40.265	1.00	0.00
ATOM	3176	CA	SER	A	411	41.895	72.385	40.981	1.00	0.00
ATOM	3177	CB	SER	A	411	42.928	73.187	41.781	1.00	0.00
ATOM	3178	OG	SER	A	411	43.264	72.551	42.995	1.00	0.00
ATOM	3179	C	SER	A	411	41.139	73.364	40.075	1.00	0.00
ATOM	3180	O	SER	A	411	40.076	73.878	40.432	1.00	0.00
ATOM	3181	N	ALA	A	412	41.708	73.626	38.907	1.00	0.00
ATOM	3182	CA	ALA	A	412	41.143	74.577	37.962	1.00	0.00
ATOM	3183	CB	ALA	A	412	42.177	74.891	36.894	1.00	0.00
ATOM	3184	C	ALA	A	412	39.827	74.136	37.319	1.00	0.00
ATOM	3185	O	ALA	A	412	38.996	74.973	36.975	1.00	0.00
ATOM	3186	N	ALA	A	413	39.629	72.831	37.172	1.00	0.00
ATOM	3187	CA	ALA	A	413	38.397	72.319	36.573	1.00	0.00
ATOM	3188	CB	ALA	A	413	38.676	71.008	35.849	1.00	0.00

Figure 1A-58

ATOM	3189	C	ALA	A	413	37.230	72.127	37.553	1.00	0.00
ATOM	3190	O	ALA	A	413	36.080	72.017	37.131	1.00	0.00
ATOM	3191	N	THR	A	414	37.504	72.084	38.853	1.00	0.00
ATOM	3192	CA	THR	A	414	36.420	71.883	39.813	1.00	0.00
ATOM	3193	CB	THR	A	414	36.909	72.012	41.269	1.00	0.00
ATOM	3194	OG1	THR	A	414	37.376	73.346	41.500	1.00	0.00
ATOM	3195	CG2	THR	A	414	38.025	71.025	41.546	1.00	0.00
ATOM	3196	C	THR	A	414	35.290	72.889	39.615	1.00	0.00
ATOM	3197	O	THR	A	414	35.530	74.064	39.327	1.00	0.00
ATOM	3198	N	PRO	A	415	34.037	72.445	39.779	1.00	0.00
ATOM	3199	CD	PRO	A	415	33.599	71.086	40.133	1.00	0.00
ATOM	3200	CA	PRO	A	415	32.885	73.334	39.619	1.00	0.00
ATOM	3201	CB	PRO	A	415	31.724	72.462	40.080	1.00	0.00
ATOM	3202	CG	PRO	A	415	32.172	71.091	39.689	1.00	0.00
ATOM	3203	C	PRO	A	415	33.043	74.580	40.489	1.00	0.00
ATOM	3204	O	PRO	A	415	32.726	75.696	40.077	1.00	0.00
ATOM	3205	N	LYS	A	416	33.552	74.371	41.696	1.00	0.00
ATOM	3206	CA	LYS	A	416	33.753	75.445	42.655	1.00	0.00
ATOM	3207	CB	LYS	A	416	34.236	74.844	43.974	1.00	0.00
ATOM	3208	CG	LYS	A	416	34.380	75.816	45.128	1.00	0.00
ATOM	3209	CD	LYS	A	416	34.674	75.058	46.421	1.00	0.00
ATOM	3210	CE	LYS	A	416	35.907	74.162	46.278	1.00	0.00
ATOM	3211	NZ	LYS	A	416	36.185	73.427	47.543	1.00	0.00
ATOM	3212	C	LYS	A	416	34.738	76.497	42.159	1.00	0.00
ATOM	3213	O	LYS	A	416	34.573	77.689	42.428	1.00	0.00
ATOM	3214	N	HIS	A	417	35.766	76.068	41.436	1.00	0.00
ATOM	3215	CA	HIS	A	417	36.741	77.024	40.938	1.00	0.00
ATOM	3216	CB	HIS	A	417	38.003	76.323	40.455	1.00	0.00
ATOM	3217	CG	HIS	A	417	39.099	77.272	40.089	1.00	0.00
ATOM	3218	CD2	HIS	A	417	39.526	77.719	38.884	1.00	0.00
ATOM	3219	ND1	HIS	A	417	39.839	77.951	41.035	1.00	0.00
ATOM	3220	CE1	HIS	A	417	40.673	78.777	40.427	1.00	0.00
ATOM	3221	NE2	HIS	A	417	40.502	78.656	39.122	1.00	0.00
ATOM	3222	C	HIS	A	417	36.142	77.831	39.793	1.00	0.00
ATOM	3223	O	HIS	A	417	36.302	79.055	39.738	1.00	0.00
ATOM	3224	N	LEU	A	418	35.461	77.140	38.879	1.00	0.00
ATOM	3225	CA	LEU	A	418	34.833	77.800	37.741	1.00	0.00
ATOM	3226	CB	LEU	A	418	34.168	76.781	36.810	1.00	0.00
ATOM	3227	CG	LEU	A	418	35.070	75.938	35.901	1.00	0.00
ATOM	3228	CD1	LEU	A	418	36.097	76.818	35.206	1.00	0.00
ATOM	3229	CD2	LEU	A	418	35.775	74.906	36.720	1.00	0.00
ATOM	3230	C	LEU	A	418	33.801	78.830	38.183	1.00	0.00
ATOM	3231	O	LEU	A	418	33.486	79.758	37.437	1.00	0.00
ATOM	3232	N	LYS	A	419	33.267	78.674	39.388	1.00	0.00
ATOM	3233	CA	LYS	A	419	32.293	79.636	39.881	1.00	0.00
ATOM	3234	CB	LYS	A	419	31.490	79.057	41.046	1.00	0.00
ATOM	3235	CG	LYS	A	419	30.549	77.918	40.665	1.00	0.00
ATOM	3236	CD	LYS	A	419	29.620	77.566	41.827	1.00	0.00
ATOM	3237	CE	LYS	A	419	30.404	77.229	43.096	1.00	0.00
ATOM	3238	NZ	LYS	A	419	29.516	76.965	44.262	1.00	0.00
ATOM	3239	C	LYS	A	419	32.996	80.913	40.334	1.00	0.00
ATOM	3240	O	LYS	A	419	32.739	81.993	39.806	1.00	0.00
ATOM	3241	N	SER	A	420	33.887	80.785	41.311	1.00	0.00
ATOM	3242	CA	SER	A	420	34.625	81.931	41.837	1.00	0.00
ATOM	3243	CB	SER	A	420	35.693	81.448	42.813	1.00	0.00
ATOM	3244	OG	SER	A	420	36.518	82.519	43.232	1.00	0.00

59/396

Figure 1A-59

ATOM	3245	C	SER	A	420	35.289	82.767	40.745	1.00	0.00
ATOM	3246	O	SER	A	420	35.671	83.916	40.966	1.00	0.00
ATOM	3247	N	ILE	A	421	35.429	82.170	39.570	1.00	0.00
ATOM	3248	CA	ILE	A	421	36.055	82.817	38.429	1.00	0.00
ATOM	3249	CB	ILE	A	421	36.910	81.769	37.647	1.00	0.00
ATOM	3250	CG2	ILE	A	421	36.661	81.860	36.155	1.00	0.00
ATOM	3251	CG1	ILE	A	421	38.391	81.970	37.969	1.00	0.00
ATOM	3252	CD1	ILE	A	421	38.718	81.932	39.449	1.00	0.00
ATOM	3253	C	ILE	A	421	34.992	83.462	37.528	1.00	0.00
ATOM	3254	O	ILE	A	421	35.309	84.269	36.650	1.00	0.00
ATOM	3255	N	GLY	A	422	33.731	83.108	37.758	1.00	0.00
ATOM	3256	CA	GLY	A	422	32.650	83.673	36.971	1.00	0.00
ATOM	3257	C	GLY	A	422	32.442	83.018	35.620	1.00	0.00
ATOM	3258	O	GLY	A	422	31.758	83.566	34.761	1.00	0.00
ATOM	3259	N	LEU	A	423	33.032	81.847	35.417	1.00	0.00
ATOM	3260	CA	LEU	A	423	32.869	81.149	34.154	1.00	0.00
ATOM	3261	CB	LEU	A	423	34.173	80.474	33.751	1.00	0.00
ATOM	3262	CG	LEU	A	423	35.190	81.451	33.166	1.00	0.00
ATOM	3263	CD1	LEU	A	423	36.399	80.690	32.649	1.00	0.00
ATOM	3264	CD2	LEU	A	423	34.535	82.238	32.037	1.00	0.00
ATOM	3265	C	LEU	A	423	31.739	80.134	34.233	1.00	0.00
ATOM	3266	O	LEU	A	423	31.285	79.612	33.218	1.00	0.00
ATOM	3267	N	LEU	A	424	31.294	79.860	35.451	1.00	0.00
ATOM	3268	CA	LEU	A	424	30.194	78.941	35.685	1.00	0.00
ATOM	3269	CB	LEU	A	424	30.703	77.608	36.233	1.00	0.00
ATOM	3270	CG	LEU	A	424	29.657	76.511	36.455	1.00	0.00
ATOM	3271	CD1	LEU	A	424	29.032	76.111	35.132	1.00	0.00
ATOM	3272	CD2	LEU	A	424	30.319	75.310	37.104	1.00	0.00
ATOM	3273	C	LEU	A	424	29.313	79.635	36.715	1.00	0.00
ATOM	3274	O	LEU	A	424	29.788	80.039	37.779	1.00	0.00
ATOM	3275	N	SER	A	425	28.037	79.794	36.388	1.00	0.00
ATOM	3276	CA	SER	A	425	27.105	80.462	37.287	1.00	0.00
ATOM	3277	CB	SER	A	425	25.814	80.806	36.553	1.00	0.00
ATOM	3278	OG	SER	A	425	25.132	79.623	36.182	1.00	0.00
ATOM	3279	C	SER	A	425	26.765	79.583	38.474	1.00	0.00
ATOM	3280	O	SER	A	425	26.935	78.364	38.427	1.00	0.00
ATOM	3281	N	PRO	A	426	26.288	80.197	39.564	1.00	0.00
ATOM	3282	CD	PRO	A	426	26.228	81.648	39.820	1.00	0.00
ATOM	3283	CA	PRO	A	426	25.920	79.437	40.760	1.00	0.00
ATOM	3284	CB	PRO	A	426	25.850	80.514	41.841	1.00	0.00
ATOM	3285	CG	PRO	A	426	25.388	81.719	41.077	1.00	0.00
ATOM	3286	C	PRO	A	426	24.577	78.743	40.532	1.00	0.00
ATOM	3287	O	PRO	A	426	23.946	78.252	41.471	1.00	0.00
ATOM	3288	N	ASP	A	427	24.156	78.710	39.269	1.00	0.00
ATOM	3289	CA	ASP	A	427	22.891	78.094	38.872	1.00	0.00
ATOM	3290	CB	ASP	A	427	22.253	78.900	37.731	1.00	0.00
ATOM	3291	CG	ASP	A	427	20.810	78.486	37.446	1.00	0.00
ATOM	3292	OD1	ASP	A	427	20.209	79.032	36.492	1.00	0.00
ATOM	3293	OD2	ASP	A	427	20.274	77.623	38.176	1.00	0.00
ATOM	3294	C	ASP	A	427	23.104	76.644	38.429	1.00	0.00
ATOM	3295	O	ASP	A	427	22.154	75.860	38.360	1.00	0.00
ATOM	3296	N	PHE	A	428	24.350	76.287	38.124	1.00	0.00
ATOM	3297	CA	PHE	A	428	24.646	74.925	37.701	1.00	0.00
ATOM	3298	CB	PHE	A	428	25.939	74.880	36.883	1.00	0.00
ATOM	3299	CG	PHE	A	428	26.226	73.531	36.286	1.00	0.00
ATOM	3300	CD1	PHE	A	428	26.700	72.488	37.080	1.00	0.00

60/396

Figure 1A-60

ATOM	3301	CD2	PHE	A	428	25.981	73.289	34.935	1.00	0.00
ATOM	3302	CE1	PHE	A	428	26.924	71.223	36.535	1.00	0.00
ATOM	3303	CE2	PHE	A	428	26.200	72.029	34.381	1.00	0.00
ATOM	3304	CZ	PHE	A	428	26.672	70.993	35.181	1.00	0.00
ATOM	3305	C	PHE	A	428	24.775	74.033	38.929	1.00	0.00
ATOM	3306	O	PHE	A	428	25.798	74.051	39.618	1.00	0.00
ATOM	3307	N	GLN	A	429	23.736	73.249	39.199	1.00	0.00
ATOM	3308	CA	GLN	A	429	23.743	72.369	40.357	1.00	0.00
ATOM	3309	CB	GLN	A	429	22.309	72.067	40.815	1.00	0.00
ATOM	3310	CG	GLN	A	429	21.526	71.092	39.938	1.00	0.00
ATOM	3311	CD	GLN	A	429	20.118	70.838	40.471	1.00	0.00
ATOM	3312	OE1	GLN	A	429	19.385	69.987	39.955	1.00	0.00
ATOM	3313	NE2	GLN	A	429	19.734	71.581	41.508	1.00	0.00
ATOM	3314	C	GLN	A	429	24.489	71.069	40.091	1.00	0.00
ATOM	3315	O	GLN	A	429	24.380	70.472	39.021	1.00	0.00
ATOM	3316	N	GLU	A	430	25.248	70.642	41.090	1.00	0.00
ATOM	3317	CA	GLU	A	430	26.026	69.423	41.003	1.00	0.00
ATOM	3318	CB	GLU	A	430	27.342	69.626	41.753	1.00	0.00
ATOM	3319	CG	GLU	A	430	28.008	70.963	41.434	1.00	0.00
ATOM	3320	CD	GLU	A	430	28.985	71.417	42.513	1.00	0.00
ATOM	3321	OE1	GLU	A	430	29.488	72.555	42.412	1.00	0.00
ATOM	3322	OE2	GLU	A	430	29.248	70.643	43.462	1.00	0.00
ATOM	3323	C	GLU	A	430	25.215	68.290	41.629	1.00	0.00
ATOM	3324	O	GLU	A	430	24.709	68.426	42.739	1.00	0.00
ATOM	3325	N	ASP	A	431	25.085	67.181	40.906	1.00	0.00
ATOM	3326	CA	ASP	A	431	24.331	66.025	41.390	1.00	0.00
ATOM	3327	CB	ASP	A	431	23.394	65.486	40.299	1.00	0.00
ATOM	3328	CG	ASP	A	431	22.535	66.563	39.673	1.00	0.00
ATOM	3329	OD1	ASP	A	431	21.744	67.196	40.402	1.00	0.00
ATOM	3330	OD2	ASP	A	431	22.648	66.774	38.446	1.00	0.00
ATOM	3331	C	ASP	A	431	25.284	64.901	41.773	1.00	0.00
ATOM	3332	O	ASP	A	431	26.478	64.959	41.491	1.00	0.00
ATOM	3333	N	ASN	A	432	24.751	63.870	42.415	1.00	0.00
ATOM	3334	CA	ASN	A	432	25.573	62.731	42.764	1.00	0.00
ATOM	3335	CB	ASN	A	432	24.840	61.820	43.773	1.00	0.00
ATOM	3336	CG	ASN	A	432	23.510	61.282	43.252	1.00	0.00
ATOM	3337	OD1	ASN	A	432	22.816	61.934	42.471	1.00	0.00
ATOM	3338	ND2	ASN	A	432	23.140	60.093	43.711	1.00	0.00
ATOM	3339	C	ASN	A	432	25.853	62.018	41.434	1.00	0.00
ATOM	3340	O	ASN	A	432	26.756	61.184	41.332	1.00	0.00
ATOM	3341	N	GLU	A	433	25.092	62.398	40.407	1.00	0.00
ATOM	3342	CA	GLU	A	433	25.226	61.822	39.074	1.00	0.00
ATOM	3343	CB	GLU	A	433	23.856	61.766	38.393	1.00	0.00
ATOM	3344	CG	GLU	A	433	23.069	60.522	38.742	1.00	0.00
ATOM	3345	CD	GLU	A	433	21.612	60.619	38.354	1.00	0.00
ATOM	3346	OE1	GLU	A	433	21.319	61.113	37.245	1.00	0.00
ATOM	3347	OE2	GLU	A	433	20.756	60.188	39.161	1.00	0.00
ATOM	3348	C	GLU	A	433	26.226	62.548	38.176	1.00	0.00
ATOM	3349	O	GLU	A	433	26.921	61.915	37.382	1.00	0.00
ATOM	3350	N	THR	A	434	26.282	63.872	38.284	1.00	0.00
ATOM	3351	CA	THR	A	434	27.226	64.651	37.497	1.00	0.00
ATOM	3352	CB	THR	A	434	26.933	66.161	37.589	1.00	0.00
ATOM	3353	OG1	THR	A	434	26.844	66.552	38.971	1.00	0.00
ATOM	3354	CG2	THR	A	434	25.624	66.496	36.861	1.00	0.00
ATOM	3355	C	THR	A	434	28.608	64.374	38.071	1.00	0.00
ATOM	3356	O	THR	A	434	29.618	64.602	37.422	1.00	0.00

61/396

Figure 1A-61

ATOM	3357	N	GLU	A	435	28.624	63.866	39.299	1.00	0.00
ATOM	3358	CA	GLU	A	435	29.848	63.516	40.009	1.00	0.00
ATOM	3359	CB	GLU	A	435	29.558	63.374	41.507	1.00	0.00
ATOM	3360	CG	GLU	A	435	30.485	64.142	42.435	1.00	0.00
ATOM	3361	CD	GLU	A	435	30.178	65.635	42.495	1.00	0.00
ATOM	3362	OE1	GLU	A	435	30.426	66.351	41.498	1.00	0.00
ATOM	3363	OE2	GLU	A	435	29.686	66.098	43.546	1.00	0.00
ATOM	3364	C	GLU	A	435	30.384	62.181	39.475	1.00	0.00
ATOM	3365	O	GLU	A	435	31.529	62.091	39.033	1.00	0.00
ATOM	3366	N	ILE	A	436	29.553	61.144	39.521	1.00	0.00
ATOM	3367	CA	ILE	A	436	29.965	59.836	39.040	1.00	0.00
ATOM	3368	CB	ILE	A	436	28.848	58.783	39.267	1.00	0.00
ATOM	3369	CG2	ILE	A	436	28.686	57.894	38.047	1.00	0.00
ATOM	3370	CG1	ILE	A	436	29.215	57.895	40.460	1.00	0.00
ATOM	3371	CD1	ILE	A	436	29.473	58.636	41.737	1.00	0.00
ATOM	3372	C	ILE	A	436	30.350	59.915	37.566	1.00	0.00
ATOM	3373	O	ILE	A	436	31.272	59.222	37.129	1.00	0.00
ATOM	3374	N	ASN	A	437	29.654	60.771	36.815	1.00	0.00
ATOM	3375	CA	ASN	A	437	29.932	60.975	35.396	1.00	0.00
ATOM	3376	CB	ASN	A	437	28.944	61.982	34.801	1.00	0.00
ATOM	3377	CG	ASN	A	437	27.795	61.324	34.072	1.00	0.00
ATOM	3378	OD1	ASN	A	437	27.576	60.108	34.173	1.00	0.00
ATOM	3379	ND2	ASN	A	437	27.036	62.131	33.338	1.00	0.00
ATOM	3380	C	ASN	A	437	31.339	61.537	35.217	1.00	0.00
ATOM	3381	O	ASN	A	437	32.039	61.226	34.242	1.00	0.00
ATOM	3382	N	PHE	A	438	31.739	62.393	36.152	1.00	0.00
ATOM	3383	CA	PHE	A	438	33.050	63.018	36.091	1.00	0.00
ATOM	3384	CB	PHE	A	438	33.075	64.263	36.990	1.00	0.00
ATOM	3385	CG	PHE	A	438	34.437	64.882	37.121	1.00	0.00
ATOM	3386	CD1	PHE	A	438	35.039	65.505	36.032	1.00	0.00
ATOM	3387	CD2	PHE	A	438	35.142	64.787	38.314	1.00	0.00
ATOM	3388	CE1	PHE	A	438	36.333	66.022	36.123	1.00	0.00
ATOM	3389	CE2	PHE	A	438	36.430	65.299	38.419	1.00	0.00
ATOM	3390	CZ	PHE	A	438	37.029	65.916	37.322	1.00	0.00
ATOM	3391	C	PHE	A	438	34.151	62.039	36.512	1.00	0.00
ATOM	3392	O	PHE	A	438	35.200	61.963	35.881	1.00	0.00
ATOM	3393	N	LEU	A	439	33.896	61.303	37.587	1.00	0.00
ATOM	3394	CA	LEU	A	439	34.836	60.327	38.119	1.00	0.00
ATOM	3395	CB	LEU	A	439	34.326	59.833	39.484	1.00	0.00
ATOM	3396	CG	LEU	A	439	35.041	60.285	40.772	1.00	0.00
ATOM	3397	CD1	LEU	A	439	35.681	61.639	40.571	1.00	0.00
ATOM	3398	CD2	LEU	A	439	34.060	60.304	41.948	1.00	0.00
ATOM	3399	C	LEU	A	439	35.054	59.148	37.156	1.00	0.00
ATOM	3400	O	LEU	A	439	36.167	58.638	37.028	1.00	0.00
ATOM	3401	N	LEU	A	440	33.988	58.723	36.482	1.00	0.00
ATOM	3402	CA	LEU	A	440	34.073	57.621	35.531	1.00	0.00
ATOM	3403	CB	LEU	A	440	32.661	57.222	35.040	1.00	0.00
ATOM	3404	CG	LEU	A	440	32.444	56.133	33.968	1.00	0.00
ATOM	3405	CD1	LEU	A	440	32.861	56.657	32.584	1.00	0.00
ATOM	3406	CD2	LEU	A	440	33.238	54.891	34.324	1.00	0.00
ATOM	3407	C	LEU	A	440	34.922	58.121	34.378	1.00	0.00
ATOM	3408	O	LEU	A	440	35.825	57.427	33.914	1.00	0.00
ATOM	3409	N	LYS	A	441	34.651	59.340	33.923	1.00	0.00
ATOM	3410	CA	LYS	A	441	35.438	59.888	32.822	1.00	0.00
ATOM	3411	CB	LYS	A	441	34.923	61.277	32.426	1.00	0.00
ATOM	3412	CG	LYS	A	441	35.698	61.888	31.256	1.00	0.00

Figure 1A-62

ATOM	3413	CD	LYS	A	441	35.147	63.244	30.839	1.00	0.00
ATOM	3414	CE	LYS	A	441	36.021	63.853	29.749	1.00	0.00
ATOM	3415	NZ	LYS	A	441	36.340	62.855	28.676	1.00	0.00
ATOM	3416	C	LYS	A	441	36.923	59.973	33.217	1.00	0.00
ATOM	3417	O	LYS	A	441	37.810	59.693	32.415	1.00	0.00
ATOM	3418	N	GLN	A	442	37.181	60.373	34.456	1.00	0.00
ATOM	3419	CA	GLN	A	442	38.550	60.481	34.967	1.00	0.00
ATOM	3420	CB	GLN	A	442	38.525	61.085	36.370	1.00	0.00
ATOM	3421	CG	GLN	A	442	38.217	62.548	36.386	1.00	0.00
ATOM	3422	CD	GLN	A	442	39.381	63.342	35.884	1.00	0.00
ATOM	3423	OE1	GLN	A	442	40.189	63.850	36.672	1.00	0.00
ATOM	3424	NE2	GLN	A	442	39.500	63.444	34.568	1.00	0.00
ATOM	3425	C	GLN	A	442	39.220	59.114	35.036	1.00	0.00
ATOM	3426	O	GLN	A	442	40.380	58.962	34.665	1.00	0.00
ATOM	3427	N	ALA	A	443	38.470	58.125	35.515	1.00	0.00
ATOM	3428	CA	ALA	A	443	38.981	56.767	35.677	1.00	0.00
ATOM	3429	CB	ALA	A	443	37.967	55.947	36.467	1.00	0.00
ATOM	3430	C	ALA	A	443	39.330	56.071	34.346	1.00	0.00
ATOM	3431	O	ALA	A	443	40.301	55.296	34.278	1.00	0.00
ATOM	3432	N	LEU	A	444	38.554	56.359	33.294	1.00	0.00
ATOM	3433	CA	LEU	A	444	38.797	55.766	31.972	1.00	0.00
ATOM	3434	CB	LEU	A	444	37.773	56.282	30.958	1.00	0.00
ATOM	3435	CG	LEU	A	444	36.585	55.435	30.495	1.00	0.00
ATOM	3436	CD1	LEU	A	444	36.361	54.222	31.351	1.00	0.00
ATOM	3437	CD2	LEU	A	444	35.374	56.340	30.445	1.00	0.00
ATOM	3438	C	LEU	A	444	40.196	56.115	31.479	1.00	0.00
ATOM	3439	O	LEU	A	444	40.847	55.325	30.779	1.00	0.00
ATOM	3440	N	THR	A	445	40.646	57.319	31.819	1.00	0.00
ATOM	3441	CA	THR	A	445	41.979	57.776	31.433	1.00	0.00
ATOM	3442	CB	THR	A	445	42.002	59.302	31.267	1.00	0.00
ATOM	3443	OG1	THR	A	445	41.014	59.678	30.303	1.00	0.00
ATOM	3444	CG2	THR	A	445	43.370	59.784	30.798	1.00	0.00
ATOM	3445	C	THR	A	445	43.023	57.401	32.498	1.00	0.00
ATOM	3446	O	THR	A	445	44.012	56.713	32.218	1.00	0.00
ATOM	3447	N	ILE	A	446	42.779	57.853	33.724	1.00	0.00
ATOM	3448	CA	ILE	A	446	43.699	57.620	34.837	1.00	0.00
ATOM	3449	CB	ILE	A	446	43.337	58.535	36.015	1.00	0.00
ATOM	3450	CG2	ILE	A	446	44.150	58.151	37.240	1.00	0.00
ATOM	3451	CG1	ILE	A	446	43.608	59.989	35.618	1.00	0.00
ATOM	3452	CD1	ILE	A	446	42.660	60.980	36.244	1.00	0.00
ATOM	3453	C	ILE	A	446	43.842	56.180	35.328	1.00	0.00
ATOM	3454	O	ILE	A	446	44.953	55.662	35.365	1.00	0.00
ATOM	3455	N	VAL	A	447	42.742	55.533	35.704	1.00	0.00
ATOM	3456	CA	VAL	A	447	42.819	54.151	36.169	1.00	0.00
ATOM	3457	CB	VAL	A	447	41.547	53.751	36.963	1.00	0.00
ATOM	3458	CG1	VAL	A	447	41.624	52.281	37.378	1.00	0.00
ATOM	3459	CG2	VAL	A	447	41.413	54.630	38.213	1.00	0.00
ATOM	3460	C	VAL	A	447	43.038	53.152	35.020	1.00	0.00
ATOM	3461	O	VAL	A	447	43.859	52.243	35.132	1.00	0.00
ATOM	3462	N	GLY	A	448	42.318	53.322	33.912	1.00	0.00
ATOM	3463	CA	GLY	A	448	42.466	52.405	32.793	1.00	0.00
ATOM	3464	C	GLY	A	448	43.890	52.221	32.286	1.00	0.00
ATOM	3465	O	GLY	A	448	44.267	51.141	31.840	1.00	0.00
ATOM	3466	N	THR	A	449	44.700	53.270	32.375	1.00	0.00
ATOM	3467	CA	THR	A	449	46.076	53.214	31.903	1.00	0.00
ATOM	3468	CB	THR	A	449	46.576	54.638	31.549	1.00	0.00

63/396

Figure 1A-63

ATOM	3469	OG1	THR	A	449	47.692	54.541	30.660	1.00	0.00
ATOM	3470	CG2	THR	A	449	47.023	55.392	32.821	1.00	0.00
ATOM	3471	C	THR	A	449	47.086	52.587	32.878	1.00	0.00
ATOM	3472	O	THR	A	449	48.182	52.190	32.468	1.00	0.00
ATOM	3473	N	LEU	A	450	46.745	52.499	34.157	1.00	0.00
ATOM	3474	CA	LEU	A	450	47.694	51.934	35.119	1.00	0.00
ATOM	3475	CB	LEU	A	450	47.169	52.097	36.548	1.00	0.00
ATOM	3476	CG	LEU	A	450	47.271	53.563	36.971	1.00	0.00
ATOM	3477	CD1	LEU	A	450	46.687	53.758	38.365	1.00	0.00
ATOM	3478	CD2	LEU	A	450	48.740	53.989	36.921	1.00	0.00
ATOM	3479	C	LEU	A	450	48.068	50.480	34.843	1.00	0.00
ATOM	3480	O	LEU	A	450	49.240	50.142	34.779	1.00	0.00
ATOM	3481	N	PRO	A	451	47.078	49.607	34.643	1.00	0.00
ATOM	3482	CD	PRO	A	451	45.616	49.733	34.745	1.00	0.00
ATOM	3483	CA	PRO	A	451	47.448	48.222	34.379	1.00	0.00
ATOM	3484	CB	PRO	A	451	46.093	47.506	34.368	1.00	0.00
ATOM	3485	CG	PRO	A	451	45.243	48.360	35.243	1.00	0.00
ATOM	3486	C	PRO	A	451	48.183	48.107	33.055	1.00	0.00
ATOM	3487	O	PRO	A	451	49.103	47.299	32.919	1.00	0.00
ATOM	3488	N	PHE	A	452	47.783	48.924	32.078	1.00	0.00
ATOM	3489	CA	PHE	A	452	48.416	48.896	30.761	1.00	0.00
ATOM	3490	CB	PHE	A	452	47.652	49.814	29.776	1.00	0.00
ATOM	3491	CG	PHE	A	452	48.353	50.004	28.452	1.00	0.00
ATOM	3492	CD1	PHE	A	452	49.488	50.822	28.356	1.00	0.00
ATOM	3493	CD2	PHE	A	452	47.913	49.329	27.315	1.00	0.00
ATOM	3494	CE1	PHE	A	452	50.175	50.959	27.159	1.00	0.00
ATOM	3495	CE2	PHE	A	452	48.592	49.457	26.097	1.00	0.00
ATOM	3496	CZ	PHE	A	452	49.731	50.276	26.020	1.00	0.00
ATOM	3497	C	PHE	A	452	49.873	49.322	30.867	1.00	0.00
ATOM	3498	O	PHE	A	452	50.760	48.706	30.281	1.00	0.00
ATOM	3499	N	THR	A	453	50.120	50.372	31.644	1.00	0.00
ATOM	3500	CA	THR	A	453	51.470	50.888	31.827	1.00	0.00
ATOM	3501	CB	THR	A	453	51.424	52.241	32.558	1.00	0.00
ATOM	3502	OG1	THR	A	453	50.611	53.134	31.796	1.00	0.00
ATOM	3503	CG2	THR	A	453	52.846	52.817	32.759	1.00	0.00
ATOM	3504	C	THR	A	453	52.361	49.923	32.600	1.00	0.00
ATOM	3505	O	THR	A	453	53.485	49.642	32.177	1.00	0.00
ATOM	3506	N	TYR	A	454	51.874	49.414	33.725	1.00	0.00
ATOM	3507	CA	TYR	A	454	52.676	48.461	34.504	1.00	0.00
ATOM	3508	CB	TYR	A	454	51.924	48.027	35.769	1.00	0.00
ATOM	3509	CG	TYR	A	454	52.481	46.763	36.397	1.00	0.00
ATOM	3510	CD1	TYR	A	454	51.671	45.652	36.600	1.00	0.00
ATOM	3511	CE1	TYR	A	454	52.185	44.464	37.132	1.00	0.00
ATOM	3512	CD2	TYR	A	454	53.829	46.667	36.748	1.00	0.00
ATOM	3513	CE2	TYR	A	454	54.359	45.489	37.286	1.00	0.00
ATOM	3514	CZ	TYR	A	454	53.528	44.389	37.473	1.00	0.00
ATOM	3515	OH	TYR	A	454	54.038	43.220	37.989	1.00	0.00
ATOM	3516	C	TYR	A	454	53.003	47.225	33.661	1.00	0.00
ATOM	3517	O	TYR	A	454	54.137	46.786	33.582	1.00	0.00
ATOM	3518	N	MET	A	455	51.998	46.663	33.012	1.00	0.00
ATOM	3519	CA	MET	A	455	52.225	45.473	32.214	1.00	0.00
ATOM	3520	CB	MET	A	455	50.894	44.967	31.659	1.00	0.00
ATOM	3521	CG	MET	A	455	50.989	43.679	30.881	1.00	0.00
ATOM	3522	SD	MET	A	455	51.115	43.962	29.117	1.00	0.00
ATOM	3523	CE	MET	A	455	52.620	43.128	28.722	1.00	0.00
ATOM	3524	C	MET	A	455	53.243	45.694	31.100	1.00	0.00

Figure 1A-64

ATOM	3525	O	MET	A	455	54.144	44.879	30.908	1.00	0.00
ATOM	3526	N	LEU	A	456	53.130	46.800	30.371	1.00	0.00
ATOM	3527	CA	LEU	A	456	54.092	47.055	29.301	1.00	0.00
ATOM	3528	CB	LEU	A	456	53.686	48.331	28.533	1.00	0.00
ATOM	3529	CG	LEU	A	456	54.557	49.283	27.679	1.00	0.00
ATOM	3530	CD1	LEU	A	456	55.941	48.774	27.495	1.00	0.00
ATOM	3531	CD2	LEU	A	456	53.867	49.527	26.309	1.00	0.00
ATOM	3532	C	LEU	A	456	55.528	47.126	29.850	1.00	0.00
ATOM	3533	O	LEU	A	456	56.418	46.451	29.343	1.00	0.00
ATOM	3534	N	GLU	A	457	55.773	47.926	30.875	1.00	0.00
ATOM	3535	CA	GLU	A	457	57.136	48.007	31.420	1.00	0.00
ATOM	3536	CB	GLU	A	457	57.228	49.107	32.471	1.00	0.00
ATOM	3537	CG	GLU	A	457	57.507	50.482	31.894	1.00	0.00
ATOM	3538	CD	GLU	A	457	58.923	50.638	31.328	1.00	0.00
ATOM	3539	OE1	GLU	A	457	59.660	51.510	31.826	1.00	0.00
ATOM	3540	OE2	GLU	A	457	59.292	49.907	30.386	1.00	0.00
ATOM	3541	C	GLU	A	457	57.647	46.690	32.023	1.00	0.00
ATOM	3542	O	GLU	A	457	58.852	46.394	31.978	1.00	0.00
ATOM	3543	N	LYS	A	458	56.736	45.907	32.590	1.00	0.00
ATOM	3544	CA	LYS	A	458	57.113	44.629	33.181	1.00	0.00
ATOM	3545	CB	LYS	A	458	55.908	43.975	33.847	1.00	0.00
ATOM	3546	CG	LYS	A	458	56.204	42.605	34.447	1.00	0.00
ATOM	3547	CD	LYS	A	458	57.196	42.693	35.604	1.00	0.00
ATOM	3548	CE	LYS	A	458	57.300	41.351	36.352	1.00	0.00
ATOM	3549	NZ	LYS	A	458	58.322	41.375	37.440	1.00	0.00
ATOM	3550	C	LYS	A	458	57.640	43.730	32.078	1.00	0.00
ATOM	3551	O	LYS	A	458	58.685	43.079	32.234	1.00	0.00
ATOM	3552	N	TRP	A	459	56.938	43.714	30.945	1.00	0.00
ATOM	3553	CA	TRP	A	459	57.370	42.903	29.830	1.00	0.00
ATOM	3554	CB	TRP	A	459	56.384	43.019	28.678	1.00	0.00
ATOM	3555	CG	TRP	A	459	56.731	42.158	27.502	1.00	0.00
ATOM	3556	CD2	TRP	A	459	57.507	42.538	26.364	1.00	0.00
ATOM	3557	CE2	TRP	A	459	57.537	41.426	25.488	1.00	0.00
ATOM	3558	CE3	TRP	A	459	58.180	43.711	25.996	1.00	0.00
ATOM	3559	CD1	TRP	A	459	56.340	40.866	27.285	1.00	0.00
ATOM	3560	NE1	TRP	A	459	56.819	40.420	26.076	1.00	0.00
ATOM	3561	CZ2	TRP	A	459	58.210	41.452	24.269	1.00	0.00
ATOM	3562	CZ3	TRP	A	459	58.852	43.746	24.784	1.00	0.00
ATOM	3563	CH2	TRP	A	459	58.862	42.620	23.929	1.00	0.00
ATOM	3564	C	TRP	A	459	58.768	43.326	29.379	1.00	0.00
ATOM	3565	O	TRP	A	459	59.628	42.477	29.127	1.00	0.00
ATOM	3566	N	ARG	A	460	59.010	44.632	29.288	1.00	0.00
ATOM	3567	CA	ARG	A	460	60.331	45.115	28.871	1.00	0.00
ATOM	3568	CB	ARG	A	460	60.341	46.627	28.685	1.00	0.00
ATOM	3569	CG	ARG	A	460	59.628	47.152	27.463	1.00	0.00
ATOM	3570	CD	ARG	A	460	59.327	48.610	27.744	1.00	0.00
ATOM	3571	NE	ARG	A	460	59.969	49.482	26.796	1.00	0.00
ATOM	3572	CZ	ARG	A	460	59.942	50.805	26.867	1.00	0.00
ATOM	3573	NH1	ARG	A	460	59.317	51.414	27.867	1.00	0.00
ATOM	3574	NH2	ARG	A	460	60.478	51.515	25.882	1.00	0.00
ATOM	3575	C	ARG	A	460	61.403	44.778	29.900	1.00	0.00
ATOM	3576	O	ARG	A	460	62.506	44.378	29.543	1.00	0.00
ATOM	3577	N	TRP	A	461	61.092	44.995	31.173	1.00	0.00
ATOM	3578	CA	TRP	A	461	62.046	44.681	32.236	1.00	0.00
ATOM	3579	CB	TRP	A	461	61.416	44.916	33.613	1.00	0.00
ATOM	3580	CG	TRP	A	461	61.320	46.372	33.969	1.00	0.00

65/396

Figure 1A-65

ATOM	3581	CD2	TRP	A	461	60.506	46.950	34.991	1.00	0.00
ATOM	3582	CE2	TRP	A	461	60.799	48.329	35.027	1.00	0.00
ATOM	3583	CE3	TRP	A	461	59.557	46.436	35.883	1.00	0.00
ATOM	3584	CD1	TRP	A	461	62.050	47.398	33.431	1.00	0.00
ATOM	3585	NE1	TRP	A	461	61.745	48.575	34.064	1.00	0.00
ATOM	3586	CZ2	TRP	A	461	60.178	49.201	35.920	1.00	0.00
ATOM	3587	CZ3	TRP	A	461	58.935	47.301	36.772	1.00	0.00
ATOM	3588	CH2	TRP	A	461	59.251	48.674	36.782	1.00	0.00
ATOM	3589	C	TRP	A	461	62.488	43.227	32.125	1.00	0.00
ATOM	3590	O	TRP	A	461	63.680	42.918	32.202	1.00	0.00
ATOM	3591	N	MET	A	462	61.513	42.347	31.913	1.00	0.00
ATOM	3592	CA	MET	A	462	61.775	40.922	31.797	1.00	0.00
ATOM	3593	CB	MET	A	462	60.465	40.145	31.839	1.00	0.00
ATOM	3594	CG	MET	A	462	59.771	40.212	33.190	1.00	0.00
ATOM	3595	SD	MET	A	462	58.189	39.343	33.127	1.00	0.00
ATOM	3596	CE	MET	A	462	58.685	37.717	33.770	1.00	0.00
ATOM	3597	C	MET	A	462	62.552	40.574	30.541	1.00	0.00
ATOM	3598	O	MET	A	462	63.429	39.694	30.565	1.00	0.00
ATOM	3599	N	VAL	A	463	62.232	41.261	29.447	1.00	0.00
ATOM	3600	CA	VAL	A	463	62.927	41.044	28.190	1.00	0.00
ATOM	3601	CB	VAL	A	463	62.319	41.901	27.052	1.00	0.00
ATOM	3602	CG1	VAL	A	463	63.278	41.969	25.880	1.00	0.00
ATOM	3603	CG2	VAL	A	463	60.989	41.294	26.594	1.00	0.00
ATOM	3604	C	VAL	A	463	64.391	41.433	28.381	1.00	0.00
ATOM	3605	O	VAL	A	463	65.289	40.678	28.014	1.00	0.00
ATOM	3606	N	PHE	A	464	64.638	42.604	28.964	1.00	0.00
ATOM	3607	CA	PHE	A	464	66.017	43.061	29.171	1.00	0.00
ATOM	3608	CB	PHE	A	464	66.032	44.505	29.706	1.00	0.00
ATOM	3609	CG	PHE	A	464	65.486	45.521	28.734	1.00	0.00
ATOM	3610	CD1	PHE	A	464	64.666	46.552	29.171	1.00	0.00
ATOM	3611	CD2	PHE	A	464	65.776	45.436	27.381	1.00	0.00
ATOM	3612	CE1	PHE	A	464	64.146	47.476	28.272	1.00	0.00
ATOM	3613	CE2	PHE	A	464	65.260	46.358	26.475	1.00	0.00
ATOM	3614	CZ	PHE	A	464	64.446	47.375	26.922	1.00	0.00
ATOM	3615	C	PHE	A	464	66.804	42.134	30.117	1.00	0.00
ATOM	3616	O	PHE	A	464	68.023	41.970	29.968	1.00	0.00
ATOM	3617	N	LYS	A	465	66.110	41.538	31.085	1.00	0.00
ATOM	3618	CA	LYS	A	465	66.757	40.615	32.019	1.00	0.00
ATOM	3619	CB	LYS	A	465	65.882	40.389	33.248	1.00	0.00
ATOM	3620	CG	LYS	A	465	65.840	41.558	34.187	1.00	0.00
ATOM	3621	CD	LYS	A	465	64.900	41.296	35.349	1.00	0.00
ATOM	3622	CE	LYS	A	465	65.064	42.382	36.399	1.00	0.00
ATOM	3623	NZ	LYS	A	465	64.220	42.162	37.598	1.00	0.00
ATOM	3624	C	LYS	A	465	67.043	39.271	31.358	1.00	0.00
ATOM	3625	O	LYS	A	465	67.866	38.509	31.835	1.00	0.00
ATOM	3626	N	GLY	A	466	66.367	38.991	30.252	1.00	0.00
ATOM	3627	CA	GLY	A	466	66.572	37.731	29.562	1.00	0.00
ATOM	3628	C	GLY	A	466	65.698	36.596	30.086	1.00	0.00
ATOM	3629	O	GLY	A	466	66.038	35.429	29.924	1.00	0.00
ATOM	3630	N	GLU	A	467	64.575	36.933	30.711	1.00	0.00
ATOM	3631	CA	GLU	A	467	63.666	35.932	31.257	1.00	0.00
ATOM	3632	CB	GLU	A	467	62.970	36.470	32.493	1.00	0.00
ATOM	3633	CG	GLU	A	467	63.900	37.130	33.469	1.00	0.00
ATOM	3634	CD	GLU	A	467	63.157	37.679	34.655	1.00	0.00
ATOM	3635	OE1	GLU	A	467	62.129	38.356	34.440	1.00	0.00
ATOM	3636	OE2	GLU	A	467	63.595	37.441	35.801	1.00	0.00

66/396

Figure 1A-66

ATOM	3637	C	GLU	A	467	62.614	35.516	30.247	1.00	0.00
ATOM	3638	O	GLU	A	467	61.820	34.617	30.512	1.00	0.00
ATOM	3639	N	ILE	A	468	62.590	36.182	29.097	1.00	0.00
ATOM	3640	CA	ILE	A	468	61.638	35.825	28.058	1.00	0.00
ATOM	3641	CB	ILE	A	468	60.559	36.902	27.848	1.00	0.00
ATOM	3642	CG2	ILE	A	468	59.558	36.406	26.821	1.00	0.00
ATOM	3643	CG1	ILE	A	468	59.837	37.215	29.158	1.00	0.00
ATOM	3644	CD1	ILE	A	468	58.935	38.443	29.067	1.00	0.00
ATOM	3645	C	ILE	A	468	62.400	35.638	26.746	1.00	0.00
ATOM	3646	O	ILE	A	468	62.746	36.603	26.068	1.00	0.00
ATOM	3647	N	PRO	A	469	62.677	34.383	26.380	1.00	0.00
ATOM	3648	CD	PRO	A	469	62.250	33.162	27.085	1.00	0.00
ATOM	3649	CA	PRO	A	469	63.401	34.056	25.147	1.00	0.00
ATOM	3650	CB	PRO	A	469	63.334	32.531	25.102	1.00	0.00
ATOM	3651	CG	PRO	A	469	63.232	32.149	26.564	1.00	0.00
ATOM	3652	C	PRO	A	469	62.718	34.679	23.937	1.00	0.00
ATOM	3653	O	PRO	A	469	61.493	34.781	23.901	1.00	0.00
ATOM	3654	N	LYS	A	470	63.510	35.085	22.950	1.00	0.00
ATOM	3655	CA	LYS	A	470	62.968	35.689	21.736	1.00	0.00
ATOM	3656	CB	LYS	A	470	64.034	35.746	20.631	1.00	0.00
ATOM	3657	CG	LYS	A	470	65.220	36.681	20.887	1.00	0.00
ATOM	3658	CD	LYS	A	470	66.242	36.588	19.741	1.00	0.00
ATOM	3659	CE	LYS	A	470	67.510	37.410	20.008	1.00	0.00
ATOM	3660	NZ	LYS	A	470	67.288	38.903	20.021	1.00	0.00
ATOM	3661	C	LYS	A	470	61.770	34.885	21.226	1.00	0.00
ATOM	3662	O	LYS	A	470	60.764	35.463	20.793	1.00	0.00
ATOM	3663	N	ASP	A	471	61.877	33.554	21.293	1.00	0.00
ATOM	3664	CA	ASP	A	471	60.805	32.678	20.809	1.00	0.00
ATOM	3665	CB	ASP	A	471	61.308	31.236	20.616	1.00	0.00
ATOM	3666	CG	ASP	A	471	61.937	30.648	21.868	1.00	0.00
ATOM	3667	OD1	ASP	A	471	61.218	30.404	22.864	1.00	0.00
ATOM	3668	OD2	ASP	A	471	63.167	30.426	21.849	1.00	0.00
ATOM	3669	C	ASP	A	471	59.531	32.676	21.634	1.00	0.00
ATOM	3670	O	ASP	A	471	58.565	32.018	21.264	1.00	0.00
ATOM	3671	N	GLN	A	472	59.521	33.423	22.738	1.00	0.00
ATOM	3672	CA	GLN	A	472	58.327	33.529	23.582	1.00	0.00
ATOM	3673	CB	GLN	A	472	58.562	32.870	24.937	1.00	0.00
ATOM	3674	CG	GLN	A	472	59.006	31.434	24.865	1.00	0.00
ATOM	3675	CD	GLN	A	472	58.521	30.657	26.063	1.00	0.00
ATOM	3676	OE1	GLN	A	472	58.861	30.974	27.210	1.00	0.00
ATOM	3677	NE2	GLN	A	472	57.702	29.639	25.808	1.00	0.00
ATOM	3678	C	GLN	A	472	57.872	34.978	23.835	1.00	0.00
ATOM	3679	O	GLN	A	472	56.972	35.209	24.647	1.00	0.00
ATOM	3680	N	TRP	A	473	58.491	35.940	23.156	1.00	0.00
ATOM	3681	CA	TRP	A	473	58.145	37.355	23.335	1.00	0.00
ATOM	3682	CB	TRP	A	473	58.899	38.224	22.335	1.00	0.00
ATOM	3683	CG	TRP	A	473	60.273	38.573	22.748	1.00	0.00
ATOM	3684	CD2	TRP	A	473	61.146	39.507	22.099	1.00	0.00
ATOM	3685	CE2	TRP	A	473	62.364	39.511	22.820	1.00	0.00
ATOM	3686	CE3	TRP	A	473	61.016	40.341	20.978	1.00	0.00
ATOM	3687	CD1	TRP	A	473	60.971	38.065	23.802	1.00	0.00
ATOM	3688	NE1	TRP	A	473	62.230	38.623	23.854	1.00	0.00
ATOM	3689	CZ2	TRP	A	473	63.448	40.317	22.457	1.00	0.00
ATOM	3690	CZ3	TRP	A	473	62.093	41.145	20.615	1.00	0.00
ATOM	3691	CH2	TRP	A	473	63.295	41.126	21.355	1.00	0.00
ATOM	3692	C	TRP	A	473	56.660	37.649	23.202	1.00	0.00

Figure 1A-67

ATOM	3693	O	TRP	A 473	56.034	38.135	24.144	1.00	0.00
ATOM	3694	N	MET	A 474	56.095	37.384	22.028	1.00	0.00
ATOM	3695	CA	MET	A 474	54.677	37.639	21.834	1.00	0.00
ATOM	3696	CB	MET	A 474	54.278	37.463	20.361	1.00	0.00
ATOM	3697	CG	MET	A 474	54.844	38.523	19.420	1.00	0.00
ATOM	3698	SD	MET	A 474	54.752	40.170	20.154	1.00	0.00
ATOM	3699	CE	MET	A 474	53.071	40.359	20.240	1.00	0.00
ATOM	3700	C	MET	A 474	53.815	36.734	22.702	1.00	0.00
ATOM	3701	O	MET	A 474	52.790	37.170	23.235	1.00	0.00
ATOM	3702	N	LYS	A 475	54.216	35.473	22.849	1.00	0.00
ATOM	3703	CA	LYS	A 475	53.434	34.562	23.666	1.00	0.00
ATOM	3704	CB	LYS	A 475	54.094	33.177	23.749	1.00	0.00
ATOM	3705	CG	LYS	A 475	53.202	32.141	24.416	1.00	0.00
ATOM	3706	CD	LYS	A 475	54.013	31.158	25.239	1.00	0.00
ATOM	3707	CE	LYS	A 475	54.082	29.778	24.589	1.00	0.00
ATOM	3708	NZ	LYS	A 475	52.761	29.067	24.629	1.00	0.00
ATOM	3709	C	LYS	A 475	53.318	35.154	25.064	1.00	0.00
ATOM	3710	O	LYS	A 475	52.222	35.265	25.615	1.00	0.00
ATOM	3711	N	LYS	A 476	54.450	35.556	25.628	1.00	0.00
ATOM	3712	CA	LYS	A 476	54.435	36.122	26.966	1.00	0.00
ATOM	3713	CB	LYS	A 476	55.862	36.274	27.495	1.00	0.00
ATOM	3714	CG	LYS	A 476	56.128	35.492	28.776	1.00	0.00
ATOM	3715	CD	LYS	A 476	55.190	35.918	29.888	1.00	0.00
ATOM	3716	CE	LYS	A 476	55.602	35.329	31.232	1.00	0.00
ATOM	3717	NZ	LYS	A 476	55.614	33.821	31.220	1.00	0.00
ATOM	3718	C	LYS	A 476	53.712	37.464	27.008	1.00	0.00
ATOM	3719	O	LYS	A 476	53.040	37.783	27.997	1.00	0.00
ATOM	3720	N	TRP	A 477	53.838	38.245	25.936	1.00	0.00
ATOM	3721	CA	TRP	A 477	53.179	39.545	25.878	1.00	0.00
ATOM	3722	CB	TRP	A 477	53.522	40.265	24.569	1.00	0.00
ATOM	3723	CG	TRP	A 477	52.726	41.525	24.298	1.00	0.00
ATOM	3724	CD2	TRP	A 477	52.988	42.838	24.811	1.00	0.00
ATOM	3725	CE2	TRP	A 477	52.041	43.717	24.220	1.00	0.00
ATOM	3726	CE3	TRP	A 477	53.930	43.361	25.709	1.00	0.00
ATOM	3727	CD1	TRP	A 477	51.657	41.655	23.449	1.00	0.00
ATOM	3728	NE1	TRP	A 477	51.246	42.966	23.394	1.00	0.00
ATOM	3729	CZ2	TRP	A 477	52.008	45.101	24.499	1.00	0.00
ATOM	3730	CZ3	TRP	A 477	53.902	44.742	25.993	1.00	0.00
ATOM	3731	CH2	TRP	A 477	52.938	45.594	25.382	1.00	0.00
ATOM	3732	C	TRP	A 477	51.677	39.377	26.000	1.00	0.00
ATOM	3733	O	TRP	A 477	51.047	40.039	26.811	1.00	0.00
ATOM	3734	N	TRP	A 478	51.098	38.488	25.200	1.00	0.00
ATOM	3735	CA	TRP	A 478	49.658	38.271	25.248	1.00	0.00
ATOM	3736	CB	TRP	A 478	49.180	37.627	23.948	1.00	0.00
ATOM	3737	CG	TRP	A 478	49.147	38.676	22.872	1.00	0.00
ATOM	3738	CD2	TRP	A 478	48.321	39.844	22.877	1.00	0.00
ATOM	3739	CE2	TRP	A 478	48.765	40.677	21.835	1.00	0.00
ATOM	3740	CE3	TRP	A 478	47.253	40.267	23.674	1.00	0.00
ATOM	3741	CD1	TRP	A 478	50.026	38.832	21.839	1.00	0.00
ATOM	3742	NE1	TRP	A 478	49.808	40.041	21.214	1.00	0.00
ATOM	3743	CZ2	TRP	A 478	48.178	41.919	21.569	1.00	0.00
ATOM	3744	CZ3	TRP	A 478	46.670	41.502	23.412	1.00	0.00
ATOM	3745	CH2	TRP	A 478	47.138	42.312	22.368	1.00	0.00
ATOM	3746	C	TRP	A 478	49.210	37.481	26.467	1.00	0.00
ATOM	3747	O	TRP	A 478	48.079	37.619	26.917	1.00	0.00
ATOM	3748	N	GLU	A 479	50.102	36.684	27.032	1.00	0.00

Figure 1A-68

ATOM	3749	CA	GLU	A	479	49.759	35.932	28.238	1.00	0.00
ATOM	3750	CB	GLU	A	479	50.901	34.973	28.591	1.00	0.00
ATOM	3751	CG	GLU	A	479	50.478	33.567	28.973	1.00	0.00
ATOM	3752	CD	GLU	A	479	51.444	32.508	28.439	1.00	0.00
ATOM	3753	OE1	GLU	A	479	52.627	32.500	28.859	1.00	0.00
ATOM	3754	OE2	GLU	A	479	51.013	31.687	27.593	1.00	0.00
ATOM	3755	C	GLU	A	479	49.604	36.991	29.333	1.00	0.00
ATOM	3756	O	GLU	A	479	48.695	36.925	30.166	1.00	0.00
ATOM	3757	N	MET	A	480	50.496	37.983	29.302	1.00	0.00
ATOM	3758	CA	MET	A	480	50.489	39.080	30.267	1.00	0.00
ATOM	3759	CB	MET	A	480	51.848	39.774	30.239	1.00	0.00
ATOM	3760	CG	MET	A	480	52.951	38.923	30.861	1.00	0.00
ATOM	3761	SD	MET	A	480	54.613	39.515	30.555	1.00	0.00
ATOM	3762	CE	MET	A	480	54.659	40.916	31.734	1.00	0.00
ATOM	3763	C	MET	A	480	49.346	40.091	30.060	1.00	0.00
ATOM	3764	O	MET	A	480	48.802	40.640	31.030	1.00	0.00
ATOM	3765	N	LYS	A	481	48.973	40.344	28.806	1.00	0.00
ATOM	3766	CA	LYS	A	481	47.858	41.256	28.552	1.00	0.00
ATOM	3767	CB	LYS	A	481	47.656	41.458	27.042	1.00	0.00
ATOM	3768	CG	LYS	A	481	48.539	42.519	26.403	1.00	0.00
ATOM	3769	CD	LYS	A	481	48.099	43.934	26.815	1.00	0.00
ATOM	3770	CE	LYS	A	481	48.725	45.003	25.922	1.00	0.00
ATOM	3771	NZ	LYS	A	481	48.167	46.366	26.211	1.00	0.00
ATOM	3772	C	LYS	A	481	46.585	40.657	29.168	1.00	0.00
ATOM	3773	O	LYS	A	481	45.817	41.357	29.839	1.00	0.00
ATOM	3774	N	ARG	A	482	46.379	39.355	28.932	1.00	0.00
ATOM	3775	CA	ARG	A	482	45.216	38.609	29.428	1.00	0.00
ATOM	3776	CB	ARG	A	482	45.226	37.169	28.894	1.00	0.00
ATOM	3777	CG	ARG	A	482	44.982	37.015	27.399	1.00	0.00
ATOM	3778	CD	ARG	A	482	45.246	35.574	26.950	1.00	0.00
ATOM	3779	NE	ARG	A	482	45.067	35.374	25.511	1.00	0.00
ATOM	3780	CZ	ARG	A	482	44.146	34.570	24.975	1.00	0.00
ATOM	3781	NH1	ARG	A	482	43.315	33.892	25.763	1.00	0.00
ATOM	3782	NH2	ARG	A	482	44.061	34.429	23.649	1.00	0.00
ATOM	3783	C	ARG	A	482	45.152	38.548	30.949	1.00	0.00
ATOM	3784	O	ARG	A	482	44.113	38.802	31.537	1.00	0.00
ATOM	3785	N	GLU	A	483	46.266	38.212	31.587	1.00	0.00
ATOM	3786	CA	GLU	A	483	46.302	38.113	33.046	1.00	0.00
ATOM	3787	CB	GLU	A	483	47.553	37.348	33.475	1.00	0.00
ATOM	3788	CG	GLU	A	483	47.409	35.855	33.366	1.00	0.00
ATOM	3789	CD	GLU	A	483	46.639	35.276	34.538	1.00	0.00
ATOM	3790	OE1	GLU	A	483	46.280	34.079	34.479	1.00	0.00
ATOM	3791	OE2	GLU	A	483	46.403	36.023	35.518	1.00	0.00
ATOM	3792	C	GLU	A	483	46.249	39.430	33.832	1.00	0.00
ATOM	3793	O	GLU	A	483	45.429	39.598	34.732	1.00	0.00
ATOM	3794	N	ILE	A	484	47.131	40.358	33.492	1.00	0.00
ATOM	3795	CA	ILE	A	484	47.229	41.634	34.203	1.00	0.00
ATOM	3796	CB	ILE	A	484	48.663	42.206	34.073	1.00	0.00
ATOM	3797	CG2	ILE	A	484	48.795	43.470	34.899	1.00	0.00
ATOM	3798	CG1	ILE	A	484	49.680	41.144	34.518	1.00	0.00
ATOM	3799	CD1	ILE	A	484	51.149	41.457	34.192	1.00	0.00
ATOM	3800	C	ILE	A	484	46.249	42.719	33.777	1.00	0.00
ATOM	3801	O	ILE	A	484	45.641	43.381	34.616	1.00	0.00
ATOM	3802	N	VAL	A	485	46.086	42.883	32.470	1.00	0.00
ATOM	3803	CA	VAL	A	485	45.224	43.929	31.935	1.00	0.00
ATOM	3804	CB	VAL	A	485	45.855	44.487	30.637	1.00	0.00

Figure 1A-69

ATOM	3805	CG1	VAL	A	485	45.172	45.807	30.202	1.00	0.00
ATOM	3806	CG2	VAL	A	485	47.341	44.682	30.865	1.00	0.00
ATOM	3807	C	VAL	A	485	43.804	43.469	31.660	1.00	0.00
ATOM	3808	O	VAL	A	485	42.876	44.270	31.658	1.00	0.00
ATOM	3809	N	GLY	A	486	43.644	42.169	31.432	1.00	0.00
ATOM	3810	CA	GLY	A	486	42.332	41.626	31.136	1.00	0.00
ATOM	3811	C	GLY	A	486	41.929	42.048	29.735	1.00	0.00
ATOM	3812	O	GLY	A	486	40.795	42.468	29.500	1.00	0.00
ATOM	3813	N	VAL	A	487	42.870	41.943	28.806	1.00	0.00
ATOM	3814	CA	VAL	A	487	42.653	42.327	27.414	1.00	0.00
ATOM	3815	CB	VAL	A	487	43.411	43.654	27.088	1.00	0.00
ATOM	3816	CG1	VAL	A	487	43.403	43.938	25.587	1.00	0.00
ATOM	3817	CG2	VAL	A	487	42.750	44.815	27.830	1.00	0.00
ATOM	3818	C	VAL	A	487	43.206	41.199	26.568	1.00	0.00
ATOM	3819	O	VAL	A	487	44.273	40.664	26.891	1.00	0.00
ATOM	3820	N	VAL	A	488	42.480	40.825	25.511	1.00	0.00
ATOM	3821	CA	VAL	A	488	42.896	39.744	24.619	1.00	0.00
ATOM	3822	CB	VAL	A	488	41.902	38.540	24.602	1.00	0.00
ATOM	3823	CG1	VAL	A	488	42.301	37.512	25.613	1.00	0.00
ATOM	3824	CG2	VAL	A	488	40.494	39.020	24.817	1.00	0.00
ATOM	3825	C	VAL	A	488	43.022	40.150	23.163	1.00	0.00
ATOM	3826	O	VAL	A	488	42.169	40.864	22.623	1.00	0.00
ATOM	3827	N	GLU	A	489	44.063	39.630	22.524	1.00	0.00
ATOM	3828	CA	GLU	A	489	44.319	39.905	21.130	1.00	0.00
ATOM	3829	CB	GLU	A	489	45.667	39.313	20.726	1.00	0.00
ATOM	3830	CG	GLU	A	489	45.707	37.792	20.630	1.00	0.00
ATOM	3831	CD	GLU	A	489	45.768	37.084	21.978	1.00	0.00
ATOM	3832	OE1	GLU	A	489	46.012	35.862	21.975	1.00	0.00
ATOM	3833	OE2	GLU	A	489	45.571	37.726	23.035	1.00	0.00
ATOM	3834	C	GLU	A	489	43.187	39.283	20.298	1.00	0.00
ATOM	3835	O	GLU	A	489	42.749	38.172	20.578	1.00	0.00
ATOM	3836	N	PRO	A	490	42.697	40.007	19.276	1.00	0.00
ATOM	3837	CD	PRO	A	490	43.095	41.402	19.016	1.00	0.00
ATOM	3838	CA	PRO	A	490	41.615	39.596	18.370	1.00	0.00
ATOM	3839	CB	PRO	A	490	41.306	40.870	17.577	1.00	0.00
ATOM	3840	CG	PRO	A	490	41.825	41.986	18.456	1.00	0.00
ATOM	3841	C	PRO	A	490	42.039	38.474	17.443	1.00	0.00
ATOM	3842	O	PRO	A	490	41.232	37.633	17.062	1.00	0.00
ATOM	3843	N	VAL	A	491	43.317	38.497	17.084	1.00	0.00
ATOM	3844	CA	VAL	A	491	43.942	37.529	16.196	1.00	0.00
ATOM	3845	CB	VAL	A	491	44.463	38.217	14.933	1.00	0.00
ATOM	3846	CG1	VAL	A	491	45.026	37.192	13.992	1.00	0.00
ATOM	3847	CG2	VAL	A	491	43.352	39.013	14.270	1.00	0.00
ATOM	3848	C	VAL	A	491	45.150	36.945	16.907	1.00	0.00
ATOM	3849	O	VAL	A	491	45.799	37.632	17.687	1.00	0.00
ATOM	3850	N	PRO	A	492	45.472	35.670	16.656	1.00	0.00
ATOM	3851	CD	PRO	A	492	44.716	34.579	16.018	1.00	0.00
ATOM	3852	CA	PRO	A	492	46.648	35.159	17.359	1.00	0.00
ATOM	3853	CB	PRO	A	492	46.476	33.640	17.263	1.00	0.00
ATOM	3854	CG	PRO	A	492	45.720	33.467	15.983	1.00	0.00
ATOM	3855	C	PRO	A	492	47.910	35.682	16.676	1.00	0.00
ATOM	3856	O	PRO	A	492	47.950	35.814	15.456	1.00	0.00
ATOM	3857	N	HIS	A	493	48.930	35.990	17.471	1.00	0.00
ATOM	3858	CA	HIS	A	493	50.185	36.521	16.952	1.00	0.00
ATOM	3859	CB	HIS	A	493	50.420	37.932	17.502	1.00	0.00
ATOM	3860	CG	HIS	A	493	49.526	38.971	16.906	1.00	0.00

70/396

Figure 1A-70

ATOM	3861	CD2	HIS	A	493	49.449	40.307	17.111	1.00	0.00
ATOM	3862	ND1	HIS	A	493	48.569	38.675	15.960	1.00	0.00
ATOM	3863	CE1	HIS	A	493	47.942	39.781	15.609	1.00	0.00
ATOM	3864	NE2	HIS	A	493	48.457	40.787	16.294	1.00	0.00
ATOM	3865	C	HIS	A	493	51.402	35.662	17.296	1.00	0.00
ATOM	3866	O	HIS	A	493	51.691	35.436	18.463	1.00	0.00
ATOM	3867	N	ASP	A	494	52.133	35.218	16.279	1.00	0.00
ATOM	3868	CA	ASP	A	494	53.321	34.409	16.519	1.00	0.00
ATOM	3869	CB	ASP	A	494	53.549	33.427	15.357	1.00	0.00
ATOM	3870	CG	ASP	A	494	53.831	34.121	14.045	1.00	0.00
ATOM	3871	OD1	ASP	A	494	53.980	33.418	13.029	1.00	0.00
ATOM	3872	OD2	ASP	A	494	53.915	35.365	14.019	1.00	0.00
ATOM	3873	C	ASP	A	494	54.535	35.326	16.732	1.00	0.00
ATOM	3874	O	ASP	A	494	54.380	36.547	16.819	1.00	0.00
ATOM	3875	N	GLU	A	495	55.734	34.748	16.809	1.00	0.00
ATOM	3876	CA	GLU	A	495	56.942	35.533	17.064	1.00	0.00
ATOM	3877	CB	GLU	A	495	58.067	34.616	17.534	1.00	0.00
ATOM	3878	CG	GLU	A	495	57.680	33.842	18.790	1.00	0.00
ATOM	3879	CD	GLU	A	495	57.229	34.747	19.915	1.00	0.00
ATOM	3880	OE1	GLU	A	495	56.392	34.318	20.742	1.00	0.00
ATOM	3881	OE2	GLU	A	495	57.725	35.889	19.981	1.00	0.00
ATOM	3882	C	GLU	A	495	57.402	36.386	15.893	1.00	0.00
ATOM	3883	O	GLU	A	495	58.441	37.045	15.943	1.00	0.00
ATOM	3884	N	THR	A	496	56.598	36.381	14.845	1.00	0.00
ATOM	3885	CA	THR	A	496	56.873	37.161	13.661	1.00	0.00
ATOM	3886	CB	THR	A	496	56.105	36.532	12.495	1.00	0.00
ATOM	3887	OG1	THR	A	496	57.015	35.720	11.729	1.00	0.00
ATOM	3888	CG2	THR	A	496	55.460	37.569	11.642	1.00	0.00
ATOM	3889	C	THR	A	496	56.478	38.631	13.923	1.00	0.00
ATOM	3890	O	THR	A	496	57.018	39.561	13.322	1.00	0.00
ATOM	3891	N	TYR	A	497	55.556	38.815	14.858	1.00	0.00
ATOM	3892	CA	TYR	A	497	55.064	40.125	15.259	1.00	0.00
ATOM	3893	CB	TYR	A	497	53.648	40.005	15.812	1.00	0.00
ATOM	3894	CG	TYR	A	497	52.571	39.690	14.814	1.00	0.00
ATOM	3895	CD1	TYR	A	497	51.709	40.683	14.357	1.00	0.00
ATOM	3896	CE1	TYR	A	497	50.657	40.383	13.511	1.00	0.00
ATOM	3897	CD2	TYR	A	497	52.357	38.382	14.384	1.00	0.00
ATOM	3898	CE2	TYR	A	497	51.311	38.070	13.541	1.00	0.00
ATOM	3899	CZ	TYR	A	497	50.459	39.071	13.113	1.00	0.00
ATOM	3900	OH	TYR	A	497	49.369	38.737	12.349	1.00	0.00
ATOM	3901	C	TYR	A	497	55.917	40.728	16.368	1.00	0.00
ATOM	3902	O	TYR	A	497	56.750	40.053	16.967	1.00	0.00
ATOM	3903	N	CYS	A	498	55.682	42.004	16.641	1.00	0.00
ATOM	3904	CA	CYS	A	498	56.359	42.710	17.718	1.00	0.00
ATOM	3905	CB	CYS	A	498	57.641	43.392	17.267	1.00	0.00
ATOM	3906	SG	CYS	A	498	58.620	43.866	18.724	1.00	0.00
ATOM	3907	C	CYS	A	498	55.372	43.762	18.155	1.00	0.00
ATOM	3908	O	CYS	A	498	55.583	44.960	17.962	1.00	0.00
ATOM	3909	N	ASP	A	499	54.281	43.297	18.744	1.00	0.00
ATOM	3910	CA	ASP	A	499	53.213	44.178	19.176	1.00	0.00
ATOM	3911	CB	ASP	A	499	52.073	43.325	19.695	1.00	0.00
ATOM	3912	CG	ASP	A	499	51.460	42.482	18.590	1.00	0.00
ATOM	3913	OD1	ASP	A	499	50.766	41.497	18.900	1.00	0.00
ATOM	3914	OD2	ASP	A	499	51.684	42.821	17.404	1.00	0.00
ATOM	3915	C	ASP	A	499	53.586	45.285	20.149	1.00	0.00
ATOM	3916	O	ASP	A	499	53.026	46.359	20.091	1.00	0.00

71/396

Figure 1A-71

ATOM	3917	N	PRO	A	500	54.530	45.043	21.064	1.00	0.00
ATOM	3918	CD	PRO	A	500	55.153	43.794	21.534	1.00	0.00
ATOM	3919	CA	PRO	A	500	54.844	46.167	21.957	1.00	0.00
ATOM	3920	CB	PRO	A	500	55.752	45.533	23.023	1.00	0.00
ATOM	3921	CG	PRO	A	500	56.315	44.321	22.344	1.00	0.00
ATOM	3922	C	PRO	A	500	55.517	47.319	21.206	1.00	0.00
ATOM	3923	O	PRO	A	500	55.285	48.493	21.508	1.00	0.00
ATOM	3924	N	ALA	A	501	56.323	46.978	20.207	1.00	0.00
ATOM	3925	CA	ALA	A	501	57.037	47.977	19.413	1.00	0.00
ATOM	3926	CB	ALA	A	501	58.091	47.297	18.559	1.00	0.00
ATOM	3927	C	ALA	A	501	56.123	48.835	18.531	1.00	0.00
ATOM	3928	O	ALA	A	501	56.558	49.851	17.975	1.00	0.00
ATOM	3929	N	SER	A	502	54.862	48.441	18.402	1.00	0.00
ATOM	3930	CA	SER	A	502	53.937	49.210	17.579	1.00	0.00
ATOM	3931	CB	SER	A	502	52.769	48.344	17.122	1.00	0.00
ATOM	3932	OG	SER	A	502	51.765	48.322	18.119	1.00	0.00
ATOM	3933	C	SER	A	502	53.405	50.386	18.395	1.00	0.00
ATOM	3934	O	SER	A	502	52.462	51.065	17.999	1.00	0.00
ATOM	3935	N	LEU	A	503	54.006	50.595	19.558	1.00	0.00
ATOM	3936	CA	LEU	A	503	53.637	51.694	20.439	1.00	0.00
ATOM	3937	CB	LEU	A	503	53.484	51.196	21.883	1.00	0.00
ATOM	3938	CG	LEU	A	503	52.682	51.995	22.917	1.00	0.00
ATOM	3939	CD1	LEU	A	503	53.507	52.133	24.176	1.00	0.00
ATOM	3940	CD2	LEU	A	503	52.288	53.361	22.389	1.00	0.00
ATOM	3941	C	LEU	A	503	54.810	52.661	20.365	1.00	0.00
ATOM	3942	O	LEU	A	503	55.963	52.236	20.466	1.00	0.00
ATOM	3943	N	PHE	A	504	54.512	53.946	20.200	1.00	0.00
ATOM	3944	CA	PHE	A	504	55.533	54.987	20.120	1.00	0.00
ATOM	3945	CB	PHE	A	504	54.877	56.366	20.292	1.00	0.00
ATOM	3946	CG	PHE	A	504	55.867	57.509	20.343	1.00	0.00
ATOM	3947	CD1	PHE	A	504	56.427	58.013	19.181	1.00	0.00
ATOM	3948	CD2	PHE	A	504	56.258	58.052	21.559	1.00	0.00
ATOM	3949	CE1	PHE	A	504	57.363	59.042	19.219	1.00	0.00
ATOM	3950	CE2	PHE	A	504	57.190	59.076	21.617	1.00	0.00
ATOM	3951	CZ	PHE	A	504	57.750	59.578	20.445	1.00	0.00
ATOM	3952	C	PHE	A	504	56.714	54.865	21.113	1.00	0.00
ATOM	3953	O	PHE	A	504	57.875	54.787	20.709	1.00	0.00
ATOM	3954	N	HIS	A	505	56.422	54.833	22.403	1.00	0.00
ATOM	3955	CA	HIS	A	505	57.492	54.781	23.400	1.00	0.00
ATOM	3956	CB	HIS	A	505	56.886	54.876	24.791	1.00	0.00
ATOM	3957	CG	HIS	A	505	55.874	55.965	24.919	1.00	0.00
ATOM	3958	CD2	HIS	A	505	54.651	56.112	24.355	1.00	0.00
ATOM	3959	ND1	HIS	A	505	56.070	57.078	25.710	1.00	0.00
ATOM	3960	CE1	HIS	A	505	55.009	57.863	25.629	1.00	0.00
ATOM	3961	NE2	HIS	A	505	54.134	57.299	24.814	1.00	0.00
ATOM	3962	C	HIS	A	505	58.400	53.564	23.306	1.00	0.00
ATOM	3963	O	HIS	A	505	59.583	53.637	23.667	1.00	0.00
ATOM	3964	N	VAL	A	506	57.865	52.449	22.808	1.00	0.00
ATOM	3965	CA	VAL	A	506	58.689	51.257	22.689	1.00	0.00
ATOM	3966	CB	VAL	A	506	57.817	49.977	22.533	1.00	0.00
ATOM	3967	CG1	VAL	A	506	58.682	48.783	22.215	1.00	0.00
ATOM	3968	CG2	VAL	A	506	57.040	49.709	23.824	1.00	0.00
ATOM	3969	C	VAL	A	506	59.649	51.387	21.515	1.00	0.00
ATOM	3970	O	VAL	A	506	60.857	51.285	21.689	1.00	0.00
ATOM	3971	N	SER	A	507	59.128	51.617	20.311	1.00	0.00
ATOM	3972	CA	SER	A	507	60.014	51.746	19.162	1.00	0.00

72/396

Figure 1A-72

ATOM	3973	CB	SER	A	507	59.217	51.654	17.852	1.00	0.00
ATOM	3974	OG	SER	A	507	58.135	52.555	17.878	1.00	0.00
ATOM	3975	C	SER	A	507	60.823	53.042	19.182	1.00	0.00
ATOM	3976	O	SER	A	507	61.775	53.179	18.420	1.00	0.00
ATOM	3977	N	ASN	A	508	60.454	53.995	20.036	1.00	0.00
ATOM	3978	CA	ASN	A	508	61.212	55.248	20.110	1.00	0.00
ATOM	3979	CB	ASN	A	508	60.265	56.453	19.982	1.00	0.00
ATOM	3980	CG	ASN	A	508	59.836	56.678	18.523	1.00	0.00
ATOM	3981	OD1	ASN	A	508	60.527	57.355	17.762	1.00	0.00
ATOM	3982	ND2	ASN	A	508	58.724	56.059	18.120	1.00	0.00
ATOM	3983	C	ASN	A	508	62.116	55.336	21.336	1.00	0.00
ATOM	3984	O	ASN	A	508	62.608	56.403	21.710	1.00	0.00
ATOM	3985	N	ASP	A	509	62.318	54.187	21.971	1.00	0.00
ATOM	3986	CA	ASP	A	509	63.249	54.074	23.083	1.00	0.00
ATOM	3987	CB	ASP	A	509	64.654	54.215	22.477	1.00	0.00
ATOM	3988	CG	ASP	A	509	65.764	54.010	23.489	1.00	0.00
ATOM	3989	OD1	ASP	A	509	65.685	53.039	24.269	1.00	0.00
ATOM	3990	OD2	ASP	A	509	66.725	54.815	23.486	1.00	0.00
ATOM	3991	C	ASP	A	509	63.077	55.001	24.301	1.00	0.00
ATOM	3992	O	ASP	A	509	64.058	55.588	24.781	1.00	0.00
ATOM	3993	N	TYR	A	510	61.848	55.122	24.808	1.00	0.00
ATOM	3994	CA	TYR	A	510	61.560	55.940	26.000	1.00	0.00
ATOM	3995	CB	TYR	A	510	60.464	56.980	25.724	1.00	0.00
ATOM	3996	CG	TYR	A	510	60.919	58.157	24.887	1.00	0.00
ATOM	3997	CD1	TYR	A	510	61.730	59.156	25.433	1.00	0.00
ATOM	3998	CE1	TYR	A	510	62.191	60.226	24.645	1.00	0.00
ATOM	3999	CD2	TYR	A	510	60.575	58.254	23.537	1.00	0.00
ATOM	4000	CE2	TYR	A	510	61.026	59.311	22.746	1.00	0.00
ATOM	4001	CZ	TYR	A	510	61.835	60.293	23.306	1.00	0.00
ATOM	4002	OH	TYR	A	510	62.283	61.338	22.527	1.00	0.00
ATOM	4003	C	TYR	A	510	61.052	55.021	27.101	1.00	0.00
ATOM	4004	O	TYR	A	510	60.280	54.090	26.834	1.00	0.00
ATOM	4005	N	SER	A	511	61.471	55.269	28.338	1.00	0.00
ATOM	4006	CA	SER	A	511	61.007	54.445	29.432	1.00	0.00
ATOM	4007	CB	SER	A	511	61.839	54.690	30.704	1.00	0.00
ATOM	4008	OG	SER	A	511	61.731	56.029	31.132	1.00	0.00
ATOM	4009	C	SER	A	511	59.546	54.801	29.650	1.00	0.00
ATOM	4010	O	SER	A	511	59.130	55.928	29.390	1.00	0.00
ATOM	4011	N	PHE	A	512	58.784	53.844	30.177	1.00	0.00
ATOM	4012	CA	PHE	A	512	57.357	54.000	30.370	1.00	0.00
ATOM	4013	CB	PHE	A	512	56.669	52.859	29.605	1.00	0.00
ATOM	4014	CG	PHE	A	512	55.326	53.218	29.012	1.00	0.00
ATOM	4015	CD1	PHE	A	512	54.153	52.628	29.494	1.00	0.00
ATOM	4016	CD2	PHE	A	512	55.238	54.106	27.945	1.00	0.00
ATOM	4017	CE1	PHE	A	512	52.896	52.916	28.913	1.00	0.00
ATOM	4018	CE2	PHE	A	512	53.997	54.404	27.354	1.00	0.00
ATOM	4019	CZ	PHE	A	512	52.819	53.804	27.842	1.00	0.00
ATOM	4020	C	PHE	A	512	56.841	54.037	31.808	1.00	0.00
ATOM	4021	O	PHE	A	512	55.772	54.591	32.052	1.00	0.00
ATOM	4022	N	ILE	A	513	57.585	53.487	32.772	1.00	0.00
ATOM	4023	CA	ILE	A	513	57.093	53.449	34.160	1.00	0.00
ATOM	4024	CB	ILE	A	513	58.097	52.691	35.090	1.00	0.00
ATOM	4025	CG2	ILE	A	513	59.253	53.605	35.488	1.00	0.00
ATOM	4026	CG1	ILE	A	513	57.379	52.217	36.357	1.00	0.00
ATOM	4027	CD1	ILE	A	513	56.249	51.213	36.113	1.00	0.00
ATOM	4028	C	ILE	A	513	56.751	54.810	34.780	1.00	0.00

Figure 1A-73

ATOM	4029	O	ILE	A	513	55.939	54.896	35.695	1.00	0.00
ATOM	4030	N	ARG	A	514	57.349	55.875	34.265	1.00	0.00
ATOM	4031	CA	ARG	A	514	57.101	57.239	34.764	1.00	0.00
ATOM	4032	CB	ARG	A	514	57.894	58.249	33.917	1.00	0.00
ATOM	4033	CG	ARG	A	514	57.480	58.251	32.439	1.00	0.00
ATOM	4034	CD	ARG	A	514	58.521	58.931	31.580	1.00	0.00
ATOM	4035	NE	ARG	A	514	58.786	60.266	32.076	1.00	0.00
ATOM	4036	CZ	ARG	A	514	59.832	61.001	31.723	1.00	0.00
ATOM	4037	NH1	ARG	A	514	60.720	60.518	30.861	1.00	0.00
ATOM	4038	NH2	ARG	A	514	59.991	62.216	32.247	1.00	0.00
ATOM	4039	C	ARG	A	514	55.628	57.622	34.747	1.00	0.00
ATOM	4040	O	ARG	A	514	55.179	58.426	35.562	1.00	0.00
ATOM	4041	N	TYR	A	515	54.860	57.058	33.818	1.00	0.00
ATOM	4042	CA	TYR	A	515	53.432	57.388	33.763	1.00	0.00
ATOM	4043	CB	TYR	A	515	52.843	56.964	32.398	1.00	0.00
ATOM	4044	CG	TYR	A	515	53.501	57.694	31.225	1.00	0.00
ATOM	4045	CD1	TYR	A	515	53.274	59.045	31.006	1.00	0.00
ATOM	4046	CE1	TYR	A	515	53.938	59.735	29.986	1.00	0.00
ATOM	4047	CD2	TYR	A	515	54.406	57.046	30.394	1.00	0.00
ATOM	4048	CE2	TYR	A	515	55.074	57.721	29.395	1.00	0.00
ATOM	4049	CZ	TYR	A	515	54.831	59.067	29.193	1.00	0.00
ATOM	4050	OH	TYR	A	515	55.475	59.722	28.173	1.00	0.00
ATOM	4051	C	TYR	A	515	52.721	56.710	34.927	1.00	0.00
ATOM	4052	O	TYR	A	515	51.674	57.163	35.392	1.00	0.00
ATOM	4053	N	TYR	A	516	53.296	55.612	35.405	1.00	0.00
ATOM	4054	CA	TYR	A	516	52.728	54.912	36.555	1.00	0.00
ATOM	4055	CB	TYR	A	516	53.332	53.506	36.701	1.00	0.00
ATOM	4056	CG	TYR	A	516	52.699	52.700	37.813	1.00	0.00
ATOM	4057	CD1	TYR	A	516	51.551	51.940	37.585	1.00	0.00
ATOM	4058	CE1	TYR	A	516	50.909	51.267	38.630	1.00	0.00
ATOM	4059	CD2	TYR	A	516	53.208	52.763	39.118	1.00	0.00
ATOM	4060	CE2	TYR	A	516	52.585	52.093	40.170	1.00	0.00
ATOM	4061	CZ	TYR	A	516	51.435	51.351	39.924	1.00	0.00
ATOM	4062	OH	TYR	A	516	50.804	50.714	40.972	1.00	0.00
ATOM	4063	C	TYR	A	516	53.046	55.730	37.810	1.00	0.00
ATOM	4064	O	TYR	A	516	52.141	56.117	38.539	1.00	0.00
ATOM	4065	N	THR	A	517	54.322	56.037	38.039	1.00	0.00
ATOM	4066	CA	THR	A	517	54.689	56.790	39.243	1.00	0.00
ATOM	4067	CB	THR	A	517	56.215	56.869	39.420	1.00	0.00
ATOM	4068	OG1	THR	A	517	56.803	57.492	38.272	1.00	0.00
ATOM	4069	CG2	THR	A	517	56.800	55.457	39.607	1.00	0.00
ATOM	4070	C	THR	A	517	54.116	58.204	39.328	1.00	0.00
ATOM	4071	O	THR	A	517	53.673	58.645	40.392	1.00	0.00
ATOM	4072	N	ARG	A	518	54.112	58.914	38.206	1.00	0.00
ATOM	4073	CA	ARG	A	518	53.584	60.278	38.171	1.00	0.00
ATOM	4074	CB	ARG	A	518	53.741	60.823	36.757	1.00	0.00
ATOM	4075	CG	ARG	A	518	53.145	62.194	36.509	1.00	0.00
ATOM	4076	CD	ARG	A	518	52.394	62.158	35.192	1.00	0.00
ATOM	4077	NE	ARG	A	518	50.971	61.934	35.398	1.00	0.00
ATOM	4078	CZ	ARG	A	518	50.119	61.586	34.439	1.00	0.00
ATOM	4079	NH1	ARG	A	518	48.830	61.414	34.733	1.00	0.00
ATOM	4080	NH2	ARG	A	518	50.559	61.386	33.199	1.00	0.00
ATOM	4081	C	ARG	A	518	52.120	60.296	38.618	1.00	0.00
ATOM	4082	O	ARG	A	518	51.697	61.166	39.393	1.00	0.00
ATOM	4083	N	THR	A	519	51.353	59.309	38.152	1.00	0.00
ATOM	4084	CA	THR	A	519	49.944	59.187	38.513	1.00	0.00

74/396

Figure 1A-74

ATOM	4085	CB	THR	A	519	49.260	57.972	37.833	1.00	0.00
ATOM	4086	OG1	THR	A	519	49.415	58.050	36.410	1.00	0.00
ATOM	4087	CG2	THR	A	519	47.788	57.941	38.204	1.00	0.00
ATOM	4088	C	THR	A	519	49.792	59.000	40.020	1.00	0.00
ATOM	4089	O	THR	A	519	48.957	59.643	40.654	1.00	0.00
ATOM	4090	N	LEU	A	520	50.567	58.097	40.605	1.00	0.00
ATOM	4091	CA	LEU	A	520	50.448	57.949	42.052	1.00	0.00
ATOM	4092	CB	LEU	A	520	51.203	56.705	42.571	1.00	0.00
ATOM	4093	CG	LEU	A	520	50.431	55.363	42.542	1.00	0.00
ATOM	4094	CD1	LEU	A	520	50.108	54.966	41.068	1.00	0.00
ATOM	4095	CD2	LEU	A	520	51.268	54.230	43.215	1.00	0.00
ATOM	4096	C	LEU	A	520	50.948	59.229	42.738	1.00	0.00
ATOM	4097	O	LEU	A	520	50.363	59.654	43.727	1.00	0.00
ATOM	4098	N	TYR	A	521	51.995	59.871	42.221	1.00	0.00
ATOM	4099	CA	TYR	A	521	52.459	61.099	42.888	1.00	0.00
ATOM	4100	CB	TYR	A	521	53.735	61.674	42.273	1.00	0.00
ATOM	4101	CG	TYR	A	521	54.931	60.790	42.296	1.00	0.00
ATOM	4102	CD1	TYR	A	521	55.107	59.828	43.297	1.00	0.00
ATOM	4103	CE1	TYR	A	521	56.241	59.032	43.318	1.00	0.00
ATOM	4104	CD2	TYR	A	521	55.918	60.924	41.324	1.00	0.00
ATOM	4105	CE2	TYR	A	521	57.040	60.138	41.343	1.00	0.00
ATOM	4106	CZ	TYR	A	521	57.201	59.196	42.338	1.00	0.00
ATOM	4107	OH	TYR	A	521	58.347	58.437	42.340	1.00	0.00
ATOM	4108	C	TYR	A	521	51.429	62.208	42.848	1.00	0.00
ATOM	4109	O	TYR	A	521	51.169	62.860	43.867	1.00	0.00
ATOM	4110	N	GLN	A	522	50.825	62.428	41.680	1.00	0.00
ATOM	4111	CA	GLN	A	522	49.855	63.509	41.588	1.00	0.00
ATOM	4112	CB	GLN	A	522	49.251	63.605	40.173	1.00	0.00
ATOM	4113	CG	GLN	A	522	48.088	62.702	39.840	1.00	0.00
ATOM	4114	CD	GLN	A	522	47.673	62.861	38.378	1.00	0.00
ATOM	4115	OE1	GLN	A	522	48.418	62.501	37.478	1.00	0.00
ATOM	4116	NE2	GLN	A	522	46.490	63.432	38.144	1.00	0.00
ATOM	4117	C	GLN	A	522	48.762	63.438	42.633	1.00	0.00
ATOM	4118	O	GLN	A	522	48.330	64.468	43.157	1.00	0.00
ATOM	4119	N	PHE	A	523	48.296	62.243	42.967	1.00	0.00
ATOM	4120	CA	PHE	A	523	47.237	62.208	43.962	1.00	0.00
ATOM	4121	CB	PHE	A	523	46.353	60.964	43.755	1.00	0.00
ATOM	4122	CG	PHE	A	523	45.489	61.055	42.513	1.00	0.00
ATOM	4123	CD1	PHE	A	523	44.490	62.019	42.423	1.00	0.00
ATOM	4124	CD2	PHE	A	523	45.720	60.226	41.414	1.00	0.00
ATOM	4125	CE1	PHE	A	523	43.725	62.169	41.255	1.00	0.00
ATOM	4126	CE2	PHE	A	523	44.960	60.365	40.235	1.00	0.00
ATOM	4127	CZ	PHE	A	523	43.958	61.347	40.163	1.00	0.00
ATOM	4128	C	PHE	A	523	47.767	62.355	45.389	1.00	0.00
ATOM	4129	O	PHE	A	523	47.063	62.846	46.263	1.00	0.00
ATOM	4130	N	GLN	A	524	49.017	61.966	45.611	1.00	0.00
ATOM	4131	CA	GLN	A	524	49.629	62.130	46.935	1.00	0.00
ATOM	4132	CB	GLN	A	524	50.993	61.423	46.999	1.00	0.00
ATOM	4133	CG	GLN	A	524	50.889	59.898	46.972	1.00	0.00
ATOM	4134	CD	GLN	A	524	52.245	59.213	47.045	1.00	0.00
ATOM	4135	OE1	GLN	A	524	52.972	59.354	48.033	1.00	0.00
ATOM	4136	NE2	GLN	A	524	52.594	58.475	46.003	1.00	0.00
ATOM	4137	C	GLN	A	524	49.798	63.638	47.153	1.00	0.00
ATOM	4138	O	GLN	A	524	49.434	64.161	48.200	1.00	0.00
ATOM	4139	N	PHE	A	525	50.327	64.333	46.145	1.00	0.00
ATOM	4140	CA	PHE	A	525	50.499	65.773	46.224	1.00	0.00

75/396

Figure 1A-75

ATOM	4141	CB	PHE	A	525	51.049	66.376	44.923	1.00	0.00
ATOM	4142	CG	PHE	A	525	52.425	65.942	44.575	1.00	0.00
ATOM	4143	CD1	PHE	A	525	53.219	65.262	45.494	1.00	0.00
ATOM	4144	CD2	PHE	A	525	52.933	66.195	43.305	1.00	0.00
ATOM	4145	CE1	PHE	A	525	54.504	64.830	45.150	1.00	0.00
ATOM	4146	CE2	PHE	A	525	54.211	65.771	42.952	1.00	0.00
ATOM	4147	CZ	PHE	A	525	55.002	65.079	43.885	1.00	0.00
ATOM	4148	C	PHE	A	525	49.153	66.412	46.456	1.00	0.00
ATOM	4149	O	PHE	A	525	49.006	67.255	47.356	1.00	0.00
ATOM	4150	N	GLN	A	526	48.164	66.031	45.642	1.00	0.00
ATOM	4151	CA	GLN	A	526	46.833	66.631	45.760	1.00	0.00
ATOM	4152	CB	GLN	A	526	45.904	66.167	44.623	1.00	0.00
ATOM	4153	CG	GLN	A	526	44.551	66.913	44.554	1.00	0.00
ATOM	4154	CD	GLN	A	526	44.708	68.395	44.180	1.00	0.00
ATOM	4155	OE1	GLN	A	526	43.727	69.101	43.919	1.00	0.00
ATOM	4156	NE2	GLN	A	526	45.944	68.863	44.153	1.00	0.00
ATOM	4157	C	GLN	A	526	46.163	66.375	47.098	1.00	0.00
ATOM	4158	O	GLN	A	526	45.517	67.273	47.645	1.00	0.00
ATOM	4159	N	GLU	A	527	46.275	65.162	47.627	1.00	0.00
ATOM	4160	CA	GLU	A	527	45.655	64.897	48.927	1.00	0.00
ATOM	4161	CB	GLU	A	527	45.778	63.419	49.320	1.00	0.00
ATOM	4162	CG	GLU	A	527	44.906	63.048	50.520	1.00	0.00
ATOM	4163	CD	GLU	A	527	44.837	61.544	50.768	1.00	0.00
ATOM	4164	OE1	GLU	A	527	45.824	60.974	51.289	1.00	0.00
ATOM	4165	OE2	GLU	A	527	43.794	60.930	50.432	1.00	0.00
ATOM	4166	C	GLU	A	527	46.364	65.779	49.960	1.00	0.00
ATOM	4167	O	GLU	A	527	45.718	66.430	50.783	1.00	0.00
ATOM	4168	N	ALA	A	528	47.690	65.839	49.868	1.00	0.00
ATOM	4169	CA	ALA	A	528	48.483	66.645	50.788	1.00	0.00
ATOM	4170	CB	ALA	A	528	49.964	66.441	50.510	1.00	0.00
ATOM	4171	C	ALA	A	528	48.139	68.131	50.734	1.00	0.00
ATOM	4172	O	ALA	A	528	47.872	68.749	51.767	1.00	0.00
ATOM	4173	N	LEU	A	529	48.144	68.721	49.542	1.00	0.00
ATOM	4174	CA	LEU	A	529	47.825	70.139	49.440	1.00	0.00
ATOM	4175	CB	LEU	A	529	48.039	70.661	48.013	1.00	0.00
ATOM	4176	CG	LEU	A	529	49.471	70.939	47.525	1.00	0.00
ATOM	4177	CD1	LEU	A	529	50.449	71.015	48.699	1.00	0.00
ATOM	4178	CD2	LEU	A	529	49.896	69.849	46.580	1.00	0.00
ATOM	4179	C	LEU	A	529	46.414	70.441	49.886	1.00	0.00
ATOM	4180	O	LEU	A	529	46.162	71.475	50.480	1.00	0.00
ATOM	4181	N	CYS	A	530	45.484	69.539	49.611	1.00	0.00
ATOM	4182	CA	CYS	A	530	44.099	69.760	50.005	1.00	0.00
ATOM	4183	C	CYS	A	530	43.891	69.643	51.514	1.00	0.00
ATOM	4184	O	CYS	A	530	43.030	70.317	52.083	1.00	0.00
ATOM	4185	CB	CYS	A	530	43.186	68.808	49.229	1.00	0.00
ATOM	4186	SG	CYS	A	530	43.188	69.309	47.479	1.00	0.00
ATOM	4187	N	GLN	A	531	44.653	68.781	52.170	1.00	0.00
ATOM	4188	CA	GLN	A	531	44.526	68.693	53.613	1.00	0.00
ATOM	4189	CB	GLN	A	531	45.292	67.485	54.171	1.00	0.00
ATOM	4190	CG	GLN	A	531	44.586	66.148	53.867	1.00	0.00
ATOM	4191	CD	GLN	A	531	45.120	64.959	54.666	1.00	0.00
ATOM	4192	OE1	GLN	A	531	44.583	63.848	54.576	1.00	0.00
ATOM	4193	NE2	GLN	A	531	46.179	65.188	55.448	1.00	0.00
ATOM	4194	C	GLN	A	531	45.091	70.003	54.160	1.00	0.00
ATOM	4195	O	GLN	A	531	44.555	70.567	55.113	1.00	0.00
ATOM	4196	N	ALA	A	532	46.151	70.502	53.522	1.00	0.00

76/396

Figure 1A-76

ATOM	4197	CA	ALA	A	532	46.780	71.748	53.935	1.00	0.00
ATOM	4198	CB	ALA	A	532	48.126	71.909	53.261	1.00	0.00
ATOM	4199	C	ALA	A	532	45.900	72.930	53.595	1.00	0.00
ATOM	4200	O	ALA	A	532	46.149	74.042	54.055	1.00	0.00
ATOM	4201	N	ALA	A	533	44.874	72.695	52.784	1.00	0.00
ATOM	4202	CA	ALA	A	533	43.963	73.760	52.401	1.00	0.00
ATOM	4203	CB	ALA	A	533	43.681	73.686	50.915	1.00	0.00
ATOM	4204	C	ALA	A	533	42.665	73.654	53.203	1.00	0.00
ATOM	4205	O	ALA	A	533	41.714	74.419	53.001	1.00	0.00
ATOM	4206	N	LYS	A	534	42.634	72.693	54.119	1.00	0.00
ATOM	4207	CA	LYS	A	534	41.467	72.477	54.968	1.00	0.00
ATOM	4208	CB	LYS	A	534	41.176	73.745	55.786	1.00	0.00
ATOM	4209	CG	LYS	A	534	42.416	74.593	56.111	1.00	0.00
ATOM	4210	CD	LYS	A	534	43.166	74.091	57.336	1.00	0.00
ATOM	4211	CE	LYS	A	534	42.507	74.590	58.626	1.00	0.00
ATOM	4212	NZ	LYS	A	534	41.071	74.181	58.760	1.00	0.00
ATOM	4213	C	LYS	A	534	40.228	72.101	54.136	1.00	0.00
ATOM	4214	O	LYS	A	534	39.104	72.482	54.482	1.00	0.00
ATOM	4215	N	HIS	A	535	40.434	71.364	53.039	1.00	0.00
ATOM	4216	CA	HIS	A	535	39.317	70.936	52.194	1.00	0.00
ATOM	4217	CB	HIS	A	535	39.824	70.216	50.945	1.00	0.00
ATOM	4218	CG	HIS	A	535	38.728	69.708	50.064	1.00	0.00
ATOM	4219	CD2	HIS	A	535	38.406	68.452	49.674	1.00	0.00
ATOM	4220	ND1	HIS	A	535	37.788	70.540	49.495	1.00	0.00
ATOM	4221	CE1	HIS	A	535	36.934	69.818	48.792	1.00	0.00
ATOM	4222	NE2	HIS	A	535	37.287	68.548	48.884	1.00	0.00
ATOM	4223	C	HIS	A	535	38.435	69.987	52.997	1.00	0.00
ATOM	4224	O	HIS	A	535	38.945	69.093	53.671	1.00	0.00
ATOM	4225	N	GLU	A	536	37.117	70.157	52.904	1.00	0.00
ATOM	4226	CA	GLU	A	536	36.198	69.330	53.679	1.00	0.00
ATOM	4227	CB	GLU	A	536	35.002	70.172	54.150	1.00	0.00
ATOM	4228	CG	GLU	A	536	35.379	71.434	54.928	1.00	0.00
ATOM	4229	CD	GLU	A	536	35.417	72.679	54.045	1.00	0.00
ATOM	4230	OE1	GLU	A	536	36.117	72.651	53.003	1.00	0.00
ATOM	4231	OE2	GLU	A	536	34.745	73.683	54.393	1.00	0.00
ATOM	4232	C	GLU	A	536	35.668	68.026	53.074	1.00	0.00
ATOM	4233	O	GLU	A	536	35.877	66.943	53.649	1.00	0.00
ATOM	4234	N	GLY	A	537	34.978	68.106	51.940	1.00	0.00
ATOM	4235	CA	GLY	A	537	34.416	66.891	51.367	1.00	0.00
ATOM	4236	C	GLY	A	537	35.317	65.978	50.546	1.00	0.00
ATOM	4237	O	GLY	A	537	36.522	65.897	50.785	1.00	0.00
ATOM	4238	N	PRO	A	538	34.747	65.275	49.555	1.00	0.00
ATOM	4239	CD	PRO	A	538	33.334	65.397	49.157	1.00	0.00
ATOM	4240	CA	PRO	A	538	35.460	64.348	48.664	1.00	0.00
ATOM	4241	CB	PRO	A	538	34.389	63.959	47.637	1.00	0.00
ATOM	4242	CG	PRO	A	538	33.114	64.116	48.386	1.00	0.00
ATOM	4243	C	PRO	A	538	36.675	65.003	47.993	1.00	0.00
ATOM	4244	O	PRO	A	538	36.590	66.120	47.480	1.00	0.00
ATOM	4245	N	LEU	A	539	37.793	64.290	47.981	1.00	0.00
ATOM	4246	CA	LEU	A	539	39.013	64.809	47.393	1.00	0.00
ATOM	4247	CB	LEU	A	539	40.104	63.725	47.417	1.00	0.00
ATOM	4248	CG	LEU	A	539	41.476	64.046	46.848	1.00	0.00
ATOM	4249	CD1	LEU	A	539	42.110	65.203	47.617	1.00	0.00
ATOM	4250	CD2	LEU	A	539	42.359	62.799	46.926	1.00	0.00
ATOM	4251	C	LEU	A	539	38.851	65.364	45.974	1.00	0.00
ATOM	4252	O	LEU	A	539	39.471	66.378	45.647	1.00	0.00

77/396

Figure 1A-77

ATOM	4253	N	HIS	A	540	38.012	64.750	45.134	1.00	0.00
ATOM	4254	CA	HIS	A	540	37.894	65.259	43.759	1.00	0.00
ATOM	4255	CB	HIS	A	540	37.176	64.256	42.835	1.00	0.00
ATOM	4256	CG	HIS	A	540	35.687	64.247	42.965	1.00	0.00
ATOM	4257	CD2	HIS	A	540	34.727	64.818	42.200	1.00	0.00
ATOM	4258	ND1	HIS	A	540	35.026	63.566	43.968	1.00	0.00
ATOM	4259	CE1	HIS	A	540	33.722	63.716	43.811	1.00	0.00
ATOM	4260	NE2	HIS	A	540	33.515	64.471	42.747	1.00	0.00
ATOM	4261	C	HIS	A	540	37.274	66.636	43.587	1.00	0.00
ATOM	4262	O	HIS	A	540	37.359	67.205	42.508	1.00	0.00
ATOM	4263	N	LYS	A	541	36.680	67.190	44.639	1.00	0.00
ATOM	4264	CA	LYS	A	541	36.051	68.510	44.548	1.00	0.00
ATOM	4265	CB	LYS	A	541	34.771	68.545	45.392	1.00	0.00
ATOM	4266	CG	LYS	A	541	33.908	67.301	45.252	1.00	0.00
ATOM	4267	CD	LYS	A	541	32.475	67.639	44.921	1.00	0.00
ATOM	4268	CE	LYS	A	541	31.833	68.463	46.006	1.00	0.00
ATOM	4269	NZ	LYS	A	541	30.392	68.709	45.733	1.00	0.00
ATOM	4270	C	LYS	A	541	36.982	69.612	45.042	1.00	0.00
ATOM	4271	O	LYS	A	541	36.620	70.786	45.054	1.00	0.00
ATOM	4272	N	CYS	A	542	38.187	69.228	45.440	1.00	0.00
ATOM	4273	CA	CYS	A	542	39.133	70.182	45.991	1.00	0.00
ATOM	4274	C	CYS	A	542	39.712	71.228	45.049	1.00	0.00
ATOM	4275	O	CYS	A	542	39.962	70.980	43.867	1.00	0.00
ATOM	4276	CB	CYS	A	542	40.272	69.434	46.686	1.00	0.00
ATOM	4277	SG	CYS	A	542	41.573	70.531	47.331	1.00	0.00
ATOM	4278	N	ASP	A	543	39.922	72.411	45.608	1.00	0.00
ATOM	4279	CA	ASP	A	543	40.503	73.529	44.883	1.00	0.00
ATOM	4280	CB	ASP	A	543	39.408	74.537	44.538	1.00	0.00
ATOM	4281	CG	ASP	A	543	39.911	75.677	43.680	1.00	0.00
ATOM	4282	OD1	ASP	A	543	41.076	75.612	43.215	1.00	0.00
ATOM	4283	OD2	ASP	A	543	39.132	76.634	43.466	1.00	0.00
ATOM	4284	C	ASP	A	543	41.522	74.131	45.854	1.00	0.00
ATOM	4285	O	ASP	A	543	41.167	74.509	46.968	1.00	0.00
ATOM	4286	N	ILE	A	544	42.785	74.211	45.459	1.00	0.00
ATOM	4287	CA	ILE	A	544	43.782	74.748	46.377	1.00	0.00
ATOM	4288	CB	ILE	A	544	45.162	74.127	46.131	1.00	0.00
ATOM	4289	CG2	ILE	A	544	45.053	72.628	46.200	1.00	0.00
ATOM	4290	CG1	ILE	A	544	45.709	74.562	44.773	1.00	0.00
ATOM	4291	CD1	ILE	A	544	47.164	74.173	44.557	1.00	0.00
ATOM	4292	C	ILE	A	544	43.950	76.266	46.392	1.00	0.00
ATOM	4293	O	ILE	A	544	44.807	76.777	47.120	1.00	0.00
ATOM	4294	N	SER	A	545	43.141	76.978	45.604	1.00	0.00
ATOM	4295	CA	SER	A	545	43.202	78.440	45.530	1.00	0.00
ATOM	4296	CB	SER	A	545	42.077	78.982	44.650	1.00	0.00
ATOM	4297	OG	SER	A	545	42.176	78.495	43.332	1.00	0.00
ATOM	4298	C	SER	A	545	43.074	79.083	46.902	1.00	0.00
ATOM	4299	O	SER	A	545	42.340	78.593	47.742	1.00	0.00
ATOM	4300	N	ASN	A	546	43.779	80.195	47.107	1.00	0.00
ATOM	4301	CA	ASN	A	546	43.748	80.938	48.369	1.00	0.00
ATOM	4302	CB	ASN	A	546	42.331	81.048	48.924	1.00	0.00
ATOM	4303	CG	ASN	A	546	41.477	82.058	48.205	1.00	0.00
ATOM	4304	OD1	ASN	A	546	40.381	82.367	48.688	1.00	0.00
ATOM	4305	ND2	ASN	A	546	41.931	82.577	47.068	1.00	0.00
ATOM	4306	C	ASN	A	546	44.586	80.316	49.471	1.00	0.00
ATOM	4307	O	ASN	A	546	44.842	80.960	50.485	1.00	0.00
ATOM	4308	N	SER	A	547	44.998	79.070	49.304	1.00	0.00

78/396

Figure 1A-78

ATOM	4309	CA	SER	A	547	45.769	78.438	50.360	1.00	0.00
ATOM	4310	CB	SER	A	547	45.437	76.950	50.428	1.00	0.00
ATOM	4311	OG	SER	A	547	46.130	76.332	51.491	1.00	0.00
ATOM	4312	C	SER	A	547	47.284	78.623	50.268	1.00	0.00
ATOM	4313	O	SER	A	547	47.964	77.885	49.552	1.00	0.00
ATOM	4314	N	THR	A	548	47.808	79.609	50.998	1.00	0.00
ATOM	4315	CA	THR	A	548	49.249	79.856	51.020	1.00	0.00
ATOM	4316	CB	THR	A	548	49.616	81.198	51.729	1.00	0.00
ATOM	4317	OG1	THR	A	548	48.935	81.282	52.980	1.00	0.00
ATOM	4318	CG2	THR	A	548	49.223	82.394	50.876	1.00	0.00
ATOM	4319	C	THR	A	548	49.890	78.696	51.778	1.00	0.00
ATOM	4320	O	THR	A	548	51.081	78.413	51.634	1.00	0.00
ATOM	4321	N	GLU	A	549	49.096	78.012	52.587	1.00	0.00
ATOM	4322	CA	GLU	A	549	49.625	76.878	53.316	1.00	0.00
ATOM	4323	CB	GLU	A	549	48.611	76.393	54.351	1.00	0.00
ATOM	4324	CG	GLU	A	549	49.263	76.039	55.666	1.00	0.00
ATOM	4325	CD	GLU	A	549	50.029	77.217	56.243	1.00	0.00
ATOM	4326	OE1	GLU	A	549	49.372	78.207	56.641	1.00	0.00
ATOM	4327	OE2	GLU	A	549	51.282	77.162	56.283	1.00	0.00
ATOM	4328	C	GLU	A	549	49.918	75.773	52.299	1.00	0.00
ATOM	4329	O	GLU	A	549	50.905	75.048	52.411	1.00	0.00
ATOM	4330	N	ALA	A	550	49.052	75.657	51.299	1.00	0.00
ATOM	4331	CA	ALA	A	550	49.223	74.653	50.257	1.00	0.00
ATOM	4332	CB	ALA	A	550	47.961	74.566	49.402	1.00	0.00
ATOM	4333	C	ALA	A	550	50.417	75.038	49.400	1.00	0.00
ATOM	4334	O	ALA	A	550	51.318	74.228	49.167	1.00	0.00
ATOM	4335	N	GLY	A	551	50.421	76.287	48.944	1.00	0.00
ATOM	4336	CA	GLY	A	551	51.510	76.788	48.122	1.00	0.00
ATOM	4337	C	GLY	A	551	52.866	76.729	48.808	1.00	0.00
ATOM	4338	O	GLY	A	551	53.897	76.596	48.144	1.00	0.00
ATOM	4339	N	GLN	A	552	52.884	76.827	50.134	1.00	0.00
ATOM	4340	CA	GLN	A	552	54.150	76.771	50.862	1.00	0.00
ATOM	4341	CB	GLN	A	552	53.979	77.239	52.309	1.00	0.00
ATOM	4342	CG	GLN	A	552	55.265	77.112	53.127	1.00	0.00
ATOM	4343	CD	GLN	A	552	56.387	78.008	52.606	1.00	0.00
ATOM	4344	OE1	GLN	A	552	56.257	79.236	52.599	1.00	0.00
ATOM	4345	NE2	GLN	A	552	57.491	77.397	52.164	1.00	0.00
ATOM	4346	C	GLN	A	552	54.685	75.347	50.858	1.00	0.00
ATOM	4347	O	GLN	A	552	55.854	75.118	50.541	1.00	0.00
ATOM	4348	N	LYS	A	553	53.828	74.394	51.222	1.00	0.00
ATOM	4349	CA	LYS	A	553	54.224	72.995	51.237	1.00	0.00
ATOM	4350	CB	LYS	A	553	53.065	72.100	51.697	1.00	0.00
ATOM	4351	CG	LYS	A	553	52.756	72.201	53.192	1.00	0.00
ATOM	4352	CD	LYS	A	553	51.901	71.037	53.661	1.00	0.00
ATOM	4353	CE	LYS	A	553	52.594	69.718	53.356	1.00	0.00
ATOM	4354	NZ	LYS	A	553	53.927	69.640	54.027	1.00	0.00
ATOM	4355	C	LYS	A	553	54.679	72.577	49.842	1.00	0.00
ATOM	4356	O	LYS	A	553	55.665	71.860	49.697	1.00	0.00
ATOM	4357	N	LEU	A	554	53.967	73.033	48.814	1.00	0.00
ATOM	4358	CA	LEU	A	554	54.331	72.683	47.450	1.00	0.00
ATOM	4359	CB	LEU	A	554	53.286	73.232	46.470	1.00	0.00
ATOM	4360	CG	LEU	A	554	53.454	72.972	44.968	1.00	0.00
ATOM	4361	CD1	LEU	A	554	53.645	71.498	44.670	1.00	0.00
ATOM	4362	CD2	LEU	A	554	52.222	73.482	44.260	1.00	0.00
ATOM	4363	C	LEU	A	554	55.712	73.252	47.134	1.00	0.00
ATOM	4364	O	LEU	A	554	56.600	72.544	46.644	1.00	0.00

Figure 1A-79

ATOM	4365	N	PHE	A	555	55.900	74.526	47.447	1.00	0.00
ATOM	4366	CA	PHE	A	555	57.168	75.195	47.177	1.00	0.00
ATOM	4367	CB	PHE	A	555	57.040	76.684	47.501	1.00	0.00
ATOM	4368	CG	PHE	A	555	58.264	77.484	47.173	1.00	0.00
ATOM	4369	CD1	PHE	A	555	59.302	77.612	48.099	1.00	0.00
ATOM	4370	CD2	PHE	A	555	58.382	78.119	45.937	1.00	0.00
ATOM	4371	CE1	PHE	A	555	60.435	78.366	47.798	1.00	0.00
ATOM	4372	CE2	PHE	A	555	59.514	78.875	45.625	1.00	0.00
ATOM	4373	CZ	PHE	A	555	60.541	79.000	46.558	1.00	0.00
ATOM	4374	C	PHE	A	555	58.396	74.607	47.882	1.00	0.00
ATOM	4375	O	PHE	A	555	59.497	74.671	47.352	1.00	0.00
ATOM	4376	N	ASN	A	556	58.222	74.040	49.067	1.00	0.00
ATOM	4377	CA	ASN	A	556	59.357	73.454	49.782	1.00	0.00
ATOM	4378	CB	ASN	A	556	58.918	72.915	51.150	1.00	0.00
ATOM	4379	CG	ASN	A	556	58.543	74.025	52.127	1.00	0.00
ATOM	4380	OD1	ASN	A	556	57.981	73.761	53.199	1.00	0.00
ATOM	4381	ND2	ASN	A	556	58.857	75.272	51.763	1.00	0.00
ATOM	4382	C	ASN	A	556	60.022	72.334	48.986	1.00	0.00
ATOM	4383	O	ASN	A	556	61.222	72.098	49.130	1.00	0.00
ATOM	4384	N	MET	A	557	59.257	71.618	48.163	1.00	0.00
ATOM	4385	CA	MET	A	557	59.874	70.561	47.367	1.00	0.00
ATOM	4386	CB	MET	A	557	58.952	69.347	47.259	1.00	0.00
ATOM	4387	CG	MET	A	557	57.889	69.475	46.234	1.00	0.00
ATOM	4388	SD	MET	A	557	58.406	68.958	44.578	1.00	0.00
ATOM	4389	CE	MET	A	557	56.781	68.804	43.854	1.00	0.00
ATOM	4390	C	MET	A	557	60.235	71.086	45.978	1.00	0.00
ATOM	4391	O	MET	A	557	61.193	70.626	45.358	1.00	0.00
ATOM	4392	N	LEU	A	558	59.472	72.065	45.505	1.00	0.00
ATOM	4393	CA	LEU	A	558	59.695	72.667	44.192	1.00	0.00
ATOM	4394	CB	LEU	A	558	58.602	73.716	43.944	1.00	0.00
ATOM	4395	CG	LEU	A	558	57.571	73.570	42.817	1.00	0.00
ATOM	4396	CD1	LEU	A	558	57.011	72.169	42.745	1.00	0.00
ATOM	4397	CD2	LEU	A	558	56.453	74.552	43.036	1.00	0.00
ATOM	4398	C	LEU	A	558	61.100	73.308	44.050	1.00	0.00
ATOM	4399	O	LEU	A	558	61.812	73.078	43.062	1.00	0.00
ATOM	4400	N	ARG	A	559	61.513	74.098	45.042	1.00	0.00
ATOM	4401	CA	ARG	A	559	62.819	74.757	44.966	1.00	0.00
ATOM	4402	CB	ARG	A	559	62.939	75.859	46.030	1.00	0.00
ATOM	4403	CG	ARG	A	559	63.000	75.333	47.444	1.00	0.00
ATOM	4404	CD	ARG	A	559	63.518	76.381	48.428	1.00	0.00
ATOM	4405	NE	ARG	A	559	64.171	75.702	49.543	1.00	0.00
ATOM	4406	CZ	ARG	A	559	65.433	75.270	49.534	1.00	0.00
ATOM	4407	NH1	ARG	A	559	66.207	75.462	48.473	1.00	0.00
ATOM	4408	NH2	ARG	A	559	65.910	74.599	50.574	1.00	0.00
ATOM	4409	C	ARG	A	559	63.986	73.782	45.097	1.00	0.00
ATOM	4410	O	ARG	A	559	65.123	74.132	44.824	1.00	0.00
ATOM	4411	N	LEU	A	560	63.710	72.550	45.500	1.00	0.00
ATOM	4412	CA	LEU	A	560	64.775	71.561	45.639	1.00	0.00
ATOM	4413	CB	LEU	A	560	64.241	70.334	46.388	1.00	0.00
ATOM	4414	CG	LEU	A	560	64.410	70.148	47.913	1.00	0.00
ATOM	4415	CD1	LEU	A	560	65.121	71.334	48.579	1.00	0.00
ATOM	4416	CD2	LEU	A	560	63.055	69.921	48.509	1.00	0.00
ATOM	4417	C	LEU	A	560	65.347	71.108	44.292	1.00	0.00
ATOM	4418	O	LEU	A	560	66.520	70.703	44.195	1.00	0.00
ATOM	4419	N	GLY	A	561	64.528	71.173	43.242	1.00	0.00
ATOM	4420	CA	GLY	A	561	65.005	70.682	41.972	1.00	0.00

80/396

Figure 1A-80

ATOM	4421	C	GLY	A	561	65.350	69.228	42.232	1.00	0.00
ATOM	4422	O	GLY	A	561	64.573	68.498	42.838	1.00	0.00
ATOM	4423	N	LYS	A	562	66.508	68.795	41.767	1.00	0.00
ATOM	4424	CA	LYS	A	562	66.943	67.429	42.007	1.00	0.00
ATOM	4425	CB	LYS	A	562	67.355	66.756	40.683	1.00	0.00
ATOM	4426	CG	LYS	A	562	66.795	65.348	40.521	1.00	0.00
ATOM	4427	CD	LYS	A	562	67.740	64.382	39.767	1.00	0.00
ATOM	4428	CE	LYS	A	562	68.108	64.878	38.373	1.00	0.00
ATOM	4429	NZ	LYS	A	562	68.888	66.145	38.432	1.00	0.00
ATOM	4430	C	LYS	A	562	68.148	67.426	42.993	1.00	0.00
ATOM	4431	O	LYS	A	562	68.983	66.526	42.951	1.00	0.00
ATOM	4432	N	SER	A	563	68.234	68.430	43.864	1.00	0.00
ATOM	4433	CA	SER	A	563	69.338	68.505	44.836	1.00	0.00
ATOM	4434	CB	SER	A	563	69.497	69.933	45.376	1.00	0.00
ATOM	4435	OG	SER	A	563	68.410	70.293	46.212	1.00	0.00
ATOM	4436	C	SER	A	563	69.166	67.546	46.023	1.00	0.00
ATOM	4437	O	SER	A	563	70.119	67.268	46.746	1.00	0.00
ATOM	4438	N	GLU	A	564	67.952	67.043	46.223	1.00	0.00
ATOM	4439	CA	GLU	A	564	67.682	66.120	47.317	1.00	0.00
ATOM	4440	CB	GLU	A	564	66.679	66.742	48.294	1.00	0.00
ATOM	4441	CG	GLU	A	564	67.220	67.947	49.059	1.00	0.00
ATOM	4442	CD	GLU	A	564	68.434	67.583	49.928	1.00	0.00
ATOM	4443	OE1	GLU	A	564	68.288	66.737	50.836	1.00	0.00
ATOM	4444	OE2	GLU	A	564	69.532	68.134	49.694	1.00	0.00
ATOM	4445	C	GLU	A	564	67.125	64.814	46.780	1.00	0.00
ATOM	4446	O	GLU	A	564	66.688	64.749	45.639	1.00	0.00
ATOM	4447	N	PRO	A	565	67.159	63.744	47.588	1.00	0.00
ATOM	4448	CD	PRO	A	565	67.801	63.594	48.909	1.00	0.00
ATOM	4449	CA	PRO	A	565	66.620	62.469	47.111	1.00	0.00
ATOM	4450	CB	PRO	A	565	66.829	61.535	48.309	1.00	0.00
ATOM	4451	CG	PRO	A	565	68.049	62.106	48.979	1.00	0.00
ATOM	4452	C	PRO	A	565	65.144	62.738	46.844	1.00	0.00
ATOM	4453	O	PRO	A	565	64.524	63.526	47.571	1.00	0.00
ATOM	4454	N	TRP	A	566	64.579	62.104	45.813	1.00	0.00
ATOM	4455	CA	TRP	A	566	63.168	62.328	45.493	1.00	0.00
ATOM	4456	CB	TRP	A	566	62.758	61.548	44.229	1.00	0.00
ATOM	4457	CG	TRP	A	566	62.840	60.049	44.353	1.00	0.00
ATOM	4458	CD2	TRP	A	566	61.823	59.173	44.860	1.00	0.00
ATOM	4459	CE2	TRP	A	566	62.313	57.862	44.752	1.00	0.00
ATOM	4460	CE3	TRP	A	566	60.546	59.374	45.392	1.00	0.00
ATOM	4461	CD1	TRP	A	566	63.876	59.260	43.978	1.00	0.00
ATOM	4462	NE1	TRP	A	566	63.572	57.941	44.212	1.00	0.00
ATOM	4463	CZ2	TRP	A	566	61.564	56.743	45.149	1.00	0.00
ATOM	4464	CZ3	TRP	A	566	59.798	58.260	45.792	1.00	0.00
ATOM	4465	CH2	TRP	A	566	60.315	56.963	45.663	1.00	0.00
ATOM	4466	C	TRP	A	566	62.329	61.884	46.686	1.00	0.00
ATOM	4467	O	TRP	A	566	61.262	62.444	46.962	1.00	0.00
ATOM	4468	N	THR	A	567	62.826	60.880	47.400	1.00	0.00
ATOM	4469	CA	THR	A	567	62.143	60.378	48.592	1.00	0.00
ATOM	4470	CB	THR	A	567	62.924	59.204	49.221	1.00	0.00
ATOM	4471	OG1	THR	A	567	64.281	59.606	49.462	1.00	0.00
ATOM	4472	CG2	THR	A	567	62.914	58.015	48.289	1.00	0.00
ATOM	4473	C	THR	A	567	61.976	61.476	49.655	1.00	0.00
ATOM	4474	O	THR	A	567	61.045	61.452	50.442	1.00	0.00
ATOM	4475	N	LEU	A	568	62.886	62.438	49.669	1.00	0.00
ATOM	4476	CA	LEU	A	568	62.827	63.541	50.618	1.00	0.00

Figure 1A-81

ATOM	4477	CB	LEU	A	568	64.246	64.070	50.892	1.00	0.00
ATOM	4478	CG	LEU	A	568	64.443	65.085	52.028	1.00	0.00
ATOM	4479	CD1	LEU	A	568	65.948	65.295	52.244	1.00	0.00
ATOM	4480	CD2	LEU	A	568	63.761	66.411	51.696	1.00	0.00
ATOM	4481	C	LEU	A	568	61.939	64.665	50.075	1.00	0.00
ATOM	4482	O	LEU	A	568	61.187	65.290	50.828	1.00	0.00
ATOM	4483	N	ALA	A	569	62.044	64.945	48.776	1.00	0.00
ATOM	4484	CA	ALA	A	569	61.205	65.981	48.170	1.00	0.00
ATOM	4485	CB	ALA	A	569	61.539	66.134	46.695	1.00	0.00
ATOM	4486	C	ALA	A	569	59.751	65.577	48.348	1.00	0.00
ATOM	4487	O	ALA	A	569	58.903	66.390	48.662	1.00	0.00
ATOM	4488	N	LEU	A	570	59.461	64.298	48.162	1.00	0.00
ATOM	4489	CA	LEU	A	570	58.095	63.799	48.340	1.00	0.00
ATOM	4490	CB	LEU	A	570	58.056	62.287	48.111	1.00	0.00
ATOM	4491	CG	LEU	A	570	56.879	61.609	47.412	1.00	0.00
ATOM	4492	CD1	LEU	A	570	56.851	60.162	47.865	1.00	0.00
ATOM	4493	CD2	LEU	A	570	55.577	62.293	47.721	1.00	0.00
ATOM	4494	C	LEU	A	570	57.682	64.067	49.776	1.00	0.00
ATOM	4495	O	LEU	A	570	56.632	64.665	50.052	1.00	0.00
ATOM	4496	N	GLU	A	571	58.521	63.596	50.696	1.00	0.00
ATOM	4497	CA	GLU	A	571	58.264	63.756	52.128	1.00	0.00
ATOM	4498	CB	GLU	A	571	59.447	63.238	52.958	1.00	0.00
ATOM	4499	CG	GLU	A	571	59.170	63.223	54.462	1.00	0.00
ATOM	4500	CD	GLU	A	571	60.369	62.760	55.276	1.00	0.00
ATOM	4501	OE1	GLU	A	571	61.389	63.483	55.310	1.00	0.00
ATOM	4502	OE2	GLU	A	571	60.291	61.664	55.871	1.00	0.00
ATOM	4503	C	GLU	A	571	57.990	65.204	52.488	1.00	0.00
ATOM	4504	O	GLU	A	571	57.095	65.490	53.274	1.00	0.00
ATOM	4505	N	ASN	A	572	58.754	66.123	51.908	1.00	0.00
ATOM	4506	CA	ASN	A	572	58.544	67.536	52.188	1.00	0.00
ATOM	4507	CB	ASN	A	572	59.546	68.379	51.401	1.00	0.00
ATOM	4508	CG	ASN	A	572	60.961	68.257	51.943	1.00	0.00
ATOM	4509	OD1	ASN	A	572	61.256	67.363	52.736	1.00	0.00
ATOM	4510	ND2	ASN	A	572	61.842	69.155	51.516	1.00	0.00
ATOM	4511	C	ASN	A	572	57.119	67.954	51.836	1.00	0.00
ATOM	4512	O	ASN	A	572	56.592	68.919	52.388	1.00	0.00
ATOM	4513	N	VAL	A	573	56.489	67.222	50.920	1.00	0.00
ATOM	4514	CA	VAL	A	573	55.127	67.548	50.511	1.00	0.00
ATOM	4515	CB	VAL	A	573	54.972	67.507	48.966	1.00	0.00
ATOM	4516	CG1	VAL	A	573	53.504	67.623	48.571	1.00	0.00
ATOM	4517	CG2	VAL	A	573	55.725	68.638	48.364	1.00	0.00
ATOM	4518	C	VAL	A	573	54.040	66.668	51.115	1.00	0.00
ATOM	4519	O	VAL	A	573	53.034	67.177	51.602	1.00	0.00
ATOM	4520	N	VAL	A	574	54.219	65.354	51.096	1.00	0.00
ATOM	4521	CA	VAL	A	574	53.157	64.511	51.624	1.00	0.00
ATOM	4522	CB	VAL	A	574	52.791	63.386	50.619	1.00	0.00
ATOM	4523	CG1	VAL	A	574	52.470	64.005	49.254	1.00	0.00
ATOM	4524	CG2	VAL	A	574	53.914	62.383	50.522	1.00	0.00
ATOM	4525	C	VAL	A	574	53.370	63.901	53.001	1.00	0.00
ATOM	4526	O	VAL	A	574	52.473	63.233	53.511	1.00	0.00
ATOM	4527	N	GLY	A	575	54.544	64.128	53.598	1.00	0.00
ATOM	4528	CA	GLY	A	575	54.824	63.599	54.927	1.00	0.00
ATOM	4529	C	GLY	A	575	55.190	62.125	54.977	1.00	0.00
ATOM	4530	O	GLY	A	575	55.107	61.493	56.029	1.00	0.00
ATOM	4531	N	ALA	A	576	55.598	61.574	53.842	1.00	0.00
ATOM	4532	CA	ALA	A	576	55.981	60.175	53.754	1.00	0.00

Figure 1A-82

ATOM	4533	CB	ALA	A	576	54.781	59.326	53.364	1.00	0.00
ATOM	4534	C	ALA	A	576	57.056	60.107	52.684	1.00	0.00
ATOM	4535	O	ALA	A	576	57.084	60.944	51.785	1.00	0.00
ATOM	4536	N	LYS	A	577	57.938	59.117	52.766	1.00	0.00
ATOM	4537	CA	LYS	A	577	59.018	59.026	51.798	1.00	0.00
ATOM	4538	CB	LYS	A	577	60.339	58.727	52.508	1.00	0.00
ATOM	4539	CG	LYS	A	577	60.381	57.411	53.238	1.00	0.00
ATOM	4540	CD	LYS	A	577	61.621	57.323	54.142	1.00	0.00
ATOM	4541	CE	LYS	A	577	61.628	58.427	55.202	1.00	0.00
ATOM	4542	NZ	LYS	A	577	62.704	58.241	56.224	1.00	0.00
ATOM	4543	C	LYS	A	577	58.800	58.032	50.676	1.00	0.00
ATOM	4544	O	LYS	A	577	59.716	57.754	49.898	1.00	0.00
ATOM	4545	N	ASN	A	578	57.608	57.467	50.583	1.00	0.00
ATOM	4546	CA	ASN	A	578	57.412	56.568	49.474	1.00	0.00
ATOM	4547	CB	ASN	A	578	57.564	55.113	49.892	1.00	0.00
ATOM	4548	CG	ASN	A	578	58.224	54.279	48.797	1.00	0.00
ATOM	4549	OD1	ASN	A	578	58.120	54.602	47.601	1.00	0.00
ATOM	4550	ND2	ASN	A	578	58.909	53.204	49.195	1.00	0.00
ATOM	4551	C	ASN	A	578	56.128	56.732	48.691	1.00	0.00
ATOM	4552	O	ASN	A	578	55.186	57.408	49.110	1.00	0.00
ATOM	4553	N	MET	A	579	56.137	56.126	47.515	1.00	0.00
ATOM	4554	CA	MET	A	579	55.004	56.132	46.614	1.00	0.00
ATOM	4555	CB	MET	A	579	55.414	55.484	45.287	1.00	0.00
ATOM	4556	CG	MET	A	579	54.310	55.368	44.242	1.00	0.00
ATOM	4557	SD	MET	A	579	54.932	54.711	42.653	1.00	0.00
ATOM	4558	CE	MET	A	579	55.443	53.033	43.149	1.00	0.00
ATOM	4559	C	MET	A	579	53.915	55.326	47.315	1.00	0.00
ATOM	4560	O	MET	A	579	54.152	54.217	47.794	1.00	0.00
ATOM	4561	N	ASN	A	580	52.730	55.913	47.394	1.00	0.00
ATOM	4562	CA	ASN	A	580	51.589	55.299	48.038	1.00	0.00
ATOM	4563	CB	ASN	A	580	51.358	55.979	49.385	1.00	0.00
ATOM	4564	CG	ASN	A	580	50.147	55.458	50.088	1.00	0.00
ATOM	4565	OD1	ASN	A	580	49.496	56.182	50.849	1.00	0.00
ATOM	4566	ND2	ASN	A	580	49.826	54.194	49.848	1.00	0.00
ATOM	4567	C	ASN	A	580	50.348	55.463	47.148	1.00	0.00
ATOM	4568	O	ASN	A	580	50.100	56.546	46.608	1.00	0.00
ATOM	4569	N	VAL	A	581	49.553	54.402	47.032	1.00	0.00
ATOM	4570	CA	VAL	A	581	48.366	54.425	46.193	1.00	0.00
ATOM	4571	CB	VAL	A	581	48.164	53.050	45.489	1.00	0.00
ATOM	4572	CG1	VAL	A	581	47.587	52.034	46.472	1.00	0.00
ATOM	4573	CG2	VAL	A	581	47.266	53.207	44.263	1.00	0.00
ATOM	4574	C	VAL	A	581	47.064	54.808	46.870	1.00	0.00
ATOM	4575	O	VAL	A	581	46.056	55.004	46.188	1.00	0.00
ATOM	4576	N	ARG	A	582	47.064	54.937	48.195	1.00	0.00
ATOM	4577	CA	ARG	A	582	45.824	55.273	48.902	1.00	0.00
ATOM	4578	CB	ARG	A	582	46.053	55.351	50.422	1.00	0.00
ATOM	4579	CG	ARG	A	582	45.780	54.037	51.152	1.00	0.00
ATOM	4580	CD	ARG	A	582	47.012	53.547	51.925	1.00	0.00
ATOM	4581	NE	ARG	A	582	47.419	54.501	52.957	1.00	0.00
ATOM	4582	CZ	ARG	A	582	48.581	54.449	53.605	1.00	0.00
ATOM	4583	NH1	ARG	A	582	49.454	53.483	53.329	1.00	0.00
ATOM	4584	NH2	ARG	A	582	48.876	55.368	54.521	1.00	0.00
ATOM	4585	C	ARG	A	582	45.142	56.552	48.440	1.00	0.00
ATOM	4586	O	ARG	A	582	43.917	56.616	48.357	1.00	0.00
ATOM	4587	N	PRO	A	583	45.921	57.606	48.174	1.00	0.00
ATOM	4588	CD	PRO	A	583	47.327	57.837	48.546	1.00	0.00

Figure 1A-83

ATOM	4589	CA	PRO	A	583	45.297	58.854	47.724	1.00	0.00
ATOM	4590	CB	PRO	A	583	46.475	59.809	47.644	1.00	0.00
ATOM	4591	CG	PRO	A	583	47.341	59.324	48.794	1.00	0.00
ATOM	4592	C	PRO	A	583	44.574	58.702	46.391	1.00	0.00
ATOM	4593	O	PRO	A	583	43.532	59.326	46.186	1.00	0.00
ATOM	4594	N	LEU	A	584	45.120	57.886	45.487	1.00	0.00
ATOM	4595	CA	LEU	A	584	44.477	57.678	44.191	1.00	0.00
ATOM	4596	CB	LEU	A	584	45.331	56.778	43.281	1.00	0.00
ATOM	4597	CG	LEU	A	584	44.665	56.300	41.980	1.00	0.00
ATOM	4598	CD1	LEU	A	584	45.661	56.230	40.836	1.00	0.00
ATOM	4599	CD2	LEU	A	584	44.044	54.929	42.216	1.00	0.00
ATOM	4600	C	LEU	A	584	43.133	57.031	44.489	1.00	0.00
ATOM	4601	O	LEU	A	584	42.099	57.459	43.985	1.00	0.00
ATOM	4602	N	LEU	A	585	43.157	56.022	45.353	1.00	0.00
ATOM	4603	CA	LEU	A	585	41.951	55.303	45.751	1.00	0.00
ATOM	4604	CB	LEU	A	585	42.322	54.146	46.681	1.00	0.00
ATOM	4605	CG	LEU	A	585	42.564	52.754	46.102	1.00	0.00
ATOM	4606	CD1	LEU	A	585	42.883	52.812	44.587	1.00	0.00
ATOM	4607	CD2	LEU	A	585	43.679	52.091	46.901	1.00	0.00
ATOM	4608	C	LEU	A	585	40.951	56.214	46.451	1.00	0.00
ATOM	4609	O	LEU	A	585	39.738	56.082	46.269	1.00	0.00
ATOM	4610	N	ASN	A	586	41.449	57.126	47.278	1.00	0.00
ATOM	4611	CA	ASN	A	586	40.538	58.029	47.972	1.00	0.00
ATOM	4612	CB	ASN	A	586	41.287	58.918	48.971	1.00	0.00
ATOM	4613	CG	ASN	A	586	41.807	58.147	50.177	1.00	0.00
ATOM	4614	OD1	ASN	A	586	42.765	58.576	50.839	1.00	0.00
ATOM	4615	ND2	ASN	A	586	41.172	57.019	50.485	1.00	0.00
ATOM	4616	C	ASN	A	586	39.839	58.910	46.953	1.00	0.00
ATOM	4617	O	ASN	A	586	38.664	59.212	47.094	1.00	0.00
ATOM	4618	N	TYR	A	587	40.576	59.332	45.934	1.00	0.00
ATOM	4619	CA	TYR	A	587	40.029	60.201	44.888	1.00	0.00
ATOM	4620	CB	TYR	A	587	41.097	60.485	43.824	1.00	0.00
ATOM	4621	CG	TYR	A	587	40.690	61.485	42.764	1.00	0.00
ATOM	4622	CD1	TYR	A	587	40.838	62.855	42.973	1.00	0.00
ATOM	4623	CE1	TYR	A	587	40.488	63.768	41.994	1.00	0.00
ATOM	4624	CD2	TYR	A	587	40.171	61.060	41.536	1.00	0.00
ATOM	4625	CE2	TYR	A	587	39.815	61.970	40.550	1.00	0.00
ATOM	4626	CZ	TYR	A	587	39.976	63.318	40.786	1.00	0.00
ATOM	4627	OH	TYR	A	587	39.625	64.219	39.811	1.00	0.00
ATOM	4628	C	TYR	A	587	38.841	59.530	44.225	1.00	0.00
ATOM	4629	O	TYR	A	587	37.780	60.142	44.048	1.00	0.00
ATOM	4630	N	PHE	A	588	39.023	58.255	43.898	1.00	0.00
ATOM	4631	CA	PHE	A	588	38.007	57.478	43.203	1.00	0.00
ATOM	4632	CB	PHE	A	588	38.693	56.520	42.223	1.00	0.00
ATOM	4633	CG	PHE	A	588	39.277	57.203	41.023	1.00	0.00
ATOM	4634	CD1	PHE	A	588	40.654	57.304	40.857	1.00	0.00
ATOM	4635	CD2	PHE	A	588	38.435	57.758	40.048	1.00	0.00
ATOM	4636	CE1	PHE	A	588	41.197	57.950	39.734	1.00	0.00
ATOM	4637	CE2	PHE	A	588	38.960	58.406	38.922	1.00	0.00
ATOM	4638	CZ	PHE	A	588	40.339	58.505	38.758	1.00	0.00
ATOM	4639	C	PHE	A	588	37.008	56.704	44.052	1.00	0.00
ATOM	4640	O	PHE	A	588	36.131	56.019	43.506	1.00	0.00
ATOM	4641	N	GLU	A	589	37.118	56.812	45.374	1.00	0.00
ATOM	4642	CA	GLU	A	589	36.198	56.097	46.256	1.00	0.00
ATOM	4643	CB	GLU	A	589	36.451	56.479	47.713	1.00	0.00
ATOM	4644	CG	GLU	A	589	37.507	55.604	48.357	1.00	0.00

Figure 1A-84

ATOM	4645	CD	GLU	A	589	37.054	54.152	48.504	1.00	0.00
ATOM	4646	OE1	GLU	A	589	37.852	53.236	48.191	1.00	0.00
ATOM	4647	OE2	GLU	A	589	35.902	53.926	48.940	1.00	0.00
ATOM	4648	C	GLU	A	589	34.707	56.250	45.934	1.00	0.00
ATOM	4649	O	GLU	A	589	33.962	55.273	45.980	1.00	0.00
ATOM	4650	N	PRO	A	590	34.246	57.475	45.630	1.00	0.00
ATOM	4651	CD	PRO	A	590	34.920	58.788	45.707	1.00	0.00
ATOM	4652	CA	PRO	A	590	32.818	57.626	45.317	1.00	0.00
ATOM	4653	CB	PRO	A	590	32.686	59.114	45.029	1.00	0.00
ATOM	4654	CG	PRO	A	590	33.765	59.727	45.927	1.00	0.00
ATOM	4655	C	PRO	A	590	32.398	56.760	44.122	1.00	0.00
ATOM	4656	O	PRO	A	590	31.316	56.168	44.127	1.00	0.00
ATOM	4657	N	LEU	A	591	33.258	56.696	43.105	1.00	0.00
ATOM	4658	CA	LEU	A	591	32.988	55.899	41.914	1.00	0.00
ATOM	4659	CB	LEU	A	591	33.959	56.269	40.786	1.00	0.00
ATOM	4660	CG	LEU	A	591	33.874	55.369	39.542	1.00	0.00
ATOM	4661	CD1	LEU	A	591	32.564	55.624	38.815	1.00	0.00
ATOM	4662	CD2	LEU	A	591	35.033	55.632	38.601	1.00	0.00
ATOM	4663	C	LEU	A	591	33.144	54.415	42.241	1.00	0.00
ATOM	4664	O	LEU	A	591	32.427	53.568	41.707	1.00	0.00
ATOM	4665	N	PHE	A	592	34.073	54.109	43.137	1.00	0.00
ATOM	4666	CA	PHE	A	592	34.338	52.734	43.507	1.00	0.00
ATOM	4667	CB	PHE	A	592	35.570	52.662	44.400	1.00	0.00
ATOM	4668	CG	PHE	A	592	35.961	51.268	44.780	1.00	0.00
ATOM	4669	CD1	PHE	A	592	36.040	50.271	43.822	1.00	0.00
ATOM	4670	CD2	PHE	A	592	36.284	50.958	46.091	1.00	0.00
ATOM	4671	CE1	PHE	A	592	36.439	48.980	44.164	1.00	0.00
ATOM	4672	CE2	PHE	A	592	36.686	49.673	46.444	1.00	0.00
ATOM	4673	CZ	PHE	A	592	36.763	48.681	45.476	1.00	0.00
ATOM	4674	C	PHE	A	592	33.163	52.064	44.195	1.00	0.00
ATOM	4675	O	PHE	A	592	32.907	50.875	43.981	1.00	0.00
ATOM	4676	N	THR	A	593	32.439	52.817	45.012	1.00	0.00
ATOM	4677	CA	THR	A	593	31.295	52.253	45.721	1.00	0.00
ATOM	4678	CB	THR	A	593	30.923	53.129	46.927	1.00	0.00
ATOM	4679	OG1	THR	A	593	30.623	54.456	46.477	1.00	0.00
ATOM	4680	CG2	THR	A	593	32.092	53.187	47.904	1.00	0.00
ATOM	4681	C	THR	A	593	30.098	52.106	44.781	1.00	0.00
ATOM	4682	O	THR	A	593	29.303	51.177	44.903	1.00	0.00
ATOM	4683	N	TRP	A	594	29.988	53.026	43.835	1.00	0.00
ATOM	4684	CA	TRP	A	594	28.920	52.997	42.847	1.00	0.00
ATOM	4685	CB	TRP	A	594	28.961	54.272	42.023	1.00	0.00
ATOM	4686	CG	TRP	A	594	27.896	54.361	40.987	1.00	0.00
ATOM	4687	CD2	TRP	A	594	28.049	54.154	39.578	1.00	0.00
ATOM	4688	CE2	TRP	A	594	26.806	54.453	38.976	1.00	0.00
ATOM	4689	CE3	TRP	A	594	29.115	53.752	38.766	1.00	0.00
ATOM	4690	CD1	TRP	A	594	26.606	54.750	41.179	1.00	0.00
ATOM	4691	NE1	TRP	A	594	25.945	54.814	39.978	1.00	0.00
ATOM	4692	CZ2	TRP	A	594	26.596	54.365	37.594	1.00	0.00
ATOM	4693	CZ3	TRP	A	594	28.910	53.665	37.392	1.00	0.00
ATOM	4694	CH2	TRP	A	594	27.654	53.974	36.819	1.00	0.00
ATOM	4695	C	TRP	A	594	29.147	51.804	41.919	1.00	0.00
ATOM	4696	O	TRP	A	594	28.218	51.072	41.584	1.00	0.00
ATOM	4697	N	LEU	A	595	30.398	51.630	41.502	1.00	0.00
ATOM	4698	CA	LEU	A	595	30.775	50.542	40.611	1.00	0.00
ATOM	4699	CB	LEU	A	595	32.284	50.606	40.343	1.00	0.00
ATOM	4700	CG	LEU	A	595	32.791	51.009	38.948	1.00	0.00

85/396

Figure 1A-85

ATOM	4701	CD1	LEU	A	595	31.810	51.917	38.254	1.00	0.00
ATOM	4702	CD2	LEU	A	595	34.156	51.688	39.074	1.00	0.00
ATOM	4703	C	LEU	A	595	30.378	49.189	41.212	1.00	0.00
ATOM	4704	O	LEU	A	595	29.684	48.399	40.568	1.00	0.00
ATOM	4705	N	LYS	A	596	30.814	48.930	42.443	1.00	0.00
ATOM	4706	CA	LYS	A	596	30.488	47.684	43.132	1.00	0.00
ATOM	4707	CB	LYS	A	596	30.937	47.759	44.591	1.00	0.00
ATOM	4708	CG	LYS	A	596	32.427	47.490	44.784	1.00	0.00
ATOM	4709	CD	LYS	A	596	33.051	48.341	45.897	1.00	0.00
ATOM	4710	CE	LYS	A	596	32.370	48.154	47.246	1.00	0.00
ATOM	4711	NZ	LYS	A	596	33.223	48.659	48.373	1.00	0.00
ATOM	4712	C	LYS	A	596	28.994	47.392	43.060	1.00	0.00
ATOM	4713	O	LYS	A	596	28.593	46.280	42.715	1.00	0.00
ATOM	4714	N	ASP	A	597	28.176	48.397	43.370	1.00	0.00
ATOM	4715	CA	ASP	A	597	26.720	48.254	43.332	1.00	0.00
ATOM	4716	CB	ASP	A	597	26.043	49.522	43.876	1.00	0.00
ATOM	4717	CG	ASP	A	597	24.527	49.394	43.945	1.00	0.00
ATOM	4718	OD1	ASP	A	597	24.033	48.516	44.689	1.00	0.00
ATOM	4719	OD2	ASP	A	597	23.826	50.170	43.254	1.00	0.00
ATOM	4720	C	ASP	A	597	26.225	47.976	41.905	1.00	0.00
ATOM	4721	O	ASP	A	597	25.277	47.213	41.706	1.00	0.00
ATOM	4722	N	GLN	A	598	26.860	48.600	40.918	1.00	0.00
ATOM	4723	CA	GLN	A	598	26.487	48.378	39.525	1.00	0.00
ATOM	4724	CB	GLN	A	598	27.206	49.366	38.604	1.00	0.00
ATOM	4725	CG	GLN	A	598	26.678	50.802	38.639	1.00	0.00
ATOM	4726	CD	GLN	A	598	25.275	50.934	38.062	1.00	0.00
ATOM	4727	OE1	GLN	A	598	24.984	50.418	36.983	1.00	0.00
ATOM	4728	NE2	GLN	A	598	24.406	51.636	38.777	1.00	0.00
ATOM	4729	C	GLN	A	598	26.857	46.958	39.108	1.00	0.00
ATOM	4730	O	GLN	A	598	26.175	46.346	38.295	1.00	0.00
ATOM	4731	N	ASN	A	599	27.945	46.440	39.668	1.00	0.00
ATOM	4732	CA	ASN	A	599	28.421	45.098	39.350	1.00	0.00
ATOM	4733	CB	ASN	A	599	29.948	45.051	39.461	1.00	0.00
ATOM	4734	CG	ASN	A	599	30.648	45.944	38.452	1.00	0.00
ATOM	4735	OD1	ASN	A	599	31.861	46.140	38.532	1.00	0.00
ATOM	4736	ND2	ASN	A	599	29.901	46.474	37.496	1.00	0.00
ATOM	4737	C	ASN	A	599	27.832	44.031	40.283	1.00	0.00
ATOM	4738	O	ASN	A	599	28.310	42.893	40.311	1.00	0.00
ATOM	4739	N	LYS	A	600	26.805	44.399	41.040	1.00	0.00
ATOM	4740	CA	LYS	A	600	26.177	43.490	42.002	1.00	0.00
ATOM	4741	CB	LYS	A	600	24.905	44.136	42.571	1.00	0.00
ATOM	4742	CG	LYS	A	600	24.336	43.466	43.822	1.00	0.00
ATOM	4743	CD	LYS	A	600	25.217	43.702	45.055	1.00	0.00
ATOM	4744	CE	LYS	A	600	24.588	43.111	46.322	1.00	0.00
ATOM	4745	NZ	LYS	A	600	25.368	43.430	47.558	1.00	0.00
ATOM	4746	C	LYS	A	600	25.831	42.131	41.401	1.00	0.00
ATOM	4747	O	LYS	A	600	25.981	41.093	42.047	1.00	0.00
ATOM	4748	N	ASN	A	601	25.381	42.142	40.154	1.00	0.00
ATOM	4749	CA	ASN	A	601	24.993	40.912	39.478	1.00	0.00
ATOM	4750	CB	ASN	A	601	23.602	41.103	38.884	1.00	0.00
ATOM	4751	CG	ASN	A	601	23.571	42.217	37.854	1.00	0.00
ATOM	4752	OD1	ASN	A	601	24.313	43.209	37.969	1.00	0.00
ATOM	4753	ND2	ASN	A	601	22.711	42.071	36.844	1.00	0.00
ATOM	4754	C	ASN	A	601	25.961	40.478	38.371	1.00	0.00
ATOM	4755	O	ASN	A	601	25.781	39.413	37.769	1.00	0.00
ATOM	4756	N	SER	A	602	26.981	41.290	38.096	1.00	0.00

86/396

Figure 1A-86

ATOM	4757	CA	SER	A	602	27.944	40.962	37.044	1.00	0.00
ATOM	4758	CB	SER	A	602	28.523	42.245	36.438	1.00	0.00
ATOM	4759	OG	SER	A	602	27.548	42.977	35.720	1.00	0.00
ATOM	4760	C	SER	A	602	29.098	40.094	37.525	1.00	0.00
ATOM	4761	O	SER	A	602	29.283	39.883	38.719	1.00	0.00
ATOM	4762	N	PHE	A	603	29.864	39.575	36.575	1.00	0.00
ATOM	4763	CA	PHE	A	603	31.037	38.786	36.907	1.00	0.00
ATOM	4764	CB	PHE	A	603	31.346	37.768	35.800	1.00	0.00
ATOM	4765	CG	PHE	A	603	32.512	36.849	36.112	1.00	0.00
ATOM	4766	CD1	PHE	A	603	33.805	37.176	35.712	1.00	0.00
ATOM	4767	CD2	PHE	A	603	32.312	35.665	36.811	1.00	0.00
ATOM	4768	CE1	PHE	A	603	34.886	36.338	36.003	1.00	0.00
ATOM	4769	CE2	PHE	A	603	33.382	34.818	37.110	1.00	0.00
ATOM	4770	CZ	PHE	A	603	34.675	35.159	36.703	1.00	0.00
ATOM	4771	C	PHE	A	603	32.153	39.825	37.008	1.00	0.00
ATOM	4772	O	PHE	A	603	32.341	40.627	36.093	1.00	0.00
ATOM	4773	N	VAL	A	604	32.854	39.844	38.136	1.00	0.00
ATOM	4774	CA	VAL	A	604	33.944	40.784	38.332	1.00	0.00
ATOM	4775	CB	VAL	A	604	33.900	41.417	39.741	1.00	0.00
ATOM	4776	CG1	VAL	A	604	34.982	42.492	39.860	1.00	0.00
ATOM	4777	CG2	VAL	A	604	32.524	42.012	39.996	1.00	0.00
ATOM	4778	C	VAL	A	604	35.262	40.037	38.156	1.00	0.00
ATOM	4779	O	VAL	A	604	35.574	39.111	38.916	1.00	0.00
ATOM	4780	N	GLY	A	605	36.036	40.440	37.151	1.00	0.00
ATOM	4781	CA	GLY	A	605	37.294	39.773	36.890	1.00	0.00
ATOM	4782	C	GLY	A	605	37.199	39.135	35.521	1.00	0.00
ATOM	4783	O	GLY	A	605	36.263	39.400	34.780	1.00	0.00
ATOM	4784	N	TRP	A	606	38.133	38.265	35.177	1.00	0.00
ATOM	4785	CA	TRP	A	606	38.081	37.682	33.854	1.00	0.00
ATOM	4786	CB	TRP	A	606	38.712	38.663	32.858	1.00	0.00
ATOM	4787	CG	TRP	A	606	40.097	39.108	33.277	1.00	0.00
ATOM	4788	CD2	TRP	A	606	40.438	40.310	33.974	1.00	0.00
ATOM	4789	CE2	TRP	A	606	41.833	40.284	34.192	1.00	0.00
ATOM	4790	CE3	TRP	A	606	39.701	41.408	34.433	1.00	0.00
ATOM	4791	CD1	TRP	A	606	41.270	38.420	33.105	1.00	0.00
ATOM	4792	NE1	TRP	A	606	42.313	39.119	33.650	1.00	0.00
ATOM	4793	CZ2	TRP	A	606	42.513	41.321	34.852	1.00	0.00
ATOM	4794	CZ3	TRP	A	606	40.377	42.440	35.088	1.00	0.00
ATOM	4795	CH2	TRP	A	606	41.769	42.386	35.290	1.00	0.00
ATOM	4796	C	TRP	A	606	38.762	36.346	33.732	1.00	0.00
ATOM	4797	O	TRP	A	606	39.615	35.988	34.539	1.00	0.00
ATOM	4798	N	SER	A	607	38.374	35.621	32.690	1.00	0.00
ATOM	4799	CA	SER	A	607	38.941	34.313	32.373	1.00	0.00
ATOM	4800	CB	SER	A	607	37.844	33.396	31.818	1.00	0.00
ATOM	4801	OG	SER	A	607	38.372	32.426	30.922	1.00	0.00
ATOM	4802	C	SER	A	607	39.983	34.571	31.299	1.00	0.00
ATOM	4803	O	SER	A	607	39.723	35.338	30.380	1.00	0.00
ATOM	4804	N	THR	A	608	41.152	33.946	31.393	1.00	0.00
ATOM	4805	CA	THR	A	608	42.174	34.177	30.378	1.00	0.00
ATOM	4806	CB	THR	A	608	43.588	34.100	30.975	1.00	0.00
ATOM	4807	OG1	THR	A	608	43.870	32.755	31.391	1.00	0.00
ATOM	4808	CG2	THR	A	608	43.707	35.051	32.157	1.00	0.00
ATOM	4809	C	THR	A	608	42.097	33.208	29.196	1.00	0.00
ATOM	4810	O	THR	A	608	42.919	33.267	28.283	1.00	0.00
ATOM	4811	N	ASP	A	609	41.094	32.334	29.210	1.00	0.00
ATOM	4812	CA	ASP	A	609	40.919	31.335	28.158	1.00	0.00

Figure 1A-87

ATOM	4813	CB	ASP	A	609	40.150	30.126	28.697	1.00	0.00
ATOM	4814	CG	ASP	A	609	40.894	29.403	29.797	1.00	0.00
ATOM	4815	OD1	ASP	A	609	40.299	28.482	30.394	1.00	0.00
ATOM	4816	OD2	ASP	A	609	42.067	29.746	30.062	1.00	0.00
ATOM	4817	C	ASP	A	609	40.178	31.862	26.949	1.00	0.00
ATOM	4818	O	ASP	A	609	40.555	31.591	25.811	1.00	0.00
ATOM	4819	N	TRP	A	610	39.116	32.612	27.195	1.00	0.00
ATOM	4820	CA	TRP	A	610	38.315	33.136	26.107	1.00	0.00
ATOM	4821	CB	TRP	A	610	37.116	33.900	26.664	1.00	0.00
ATOM	4822	CG	TRP	A	610	36.186	34.361	25.587	1.00	0.00
ATOM	4823	CD2	TRP	A	610	36.175	35.651	24.953	1.00	0.00
ATOM	4824	CE2	TRP	A	610	35.148	35.629	23.984	1.00	0.00
ATOM	4825	CE3	TRP	A	610	36.933	36.821	25.110	1.00	0.00
ATOM	4826	CD1	TRP	A	610	35.198	33.632	24.991	1.00	0.00
ATOM	4827	NE1	TRP	A	610	34.571	34.387	24.028	1.00	0.00
ATOM	4828	CZ2	TRP	A	610	34.854	36.735	23.173	1.00	0.00
ATOM	4829	CZ3	TRP	A	610	36.641	37.928	24.299	1.00	0.00
ATOM	4830	CH2	TRP	A	610	35.611	37.872	23.348	1.00	0.00
ATOM	4831	C	TRP	A	610	39.070	34.035	25.131	1.00	0.00
ATOM	4832	O	TRP	A	610	39.989	34.775	25.510	1.00	0.00
ATOM	4833	N	SER	A	611	38.682	33.948	23.862	1.00	0.00
ATOM	4834	CA	SER	A	611	39.270	34.773	22.818	1.00	0.00
ATOM	4835	CB	SER	A	611	40.571	34.158	22.280	1.00	0.00
ATOM	4836	OG	SER	A	611	40.349	32.913	21.654	1.00	0.00
ATOM	4837	C	SER	A	611	38.233	34.899	21.712	1.00	0.00
ATOM	4838	O	SER	A	611	37.384	34.023	21.548	1.00	0.00
ATOM	4839	N	PRO	A	612	38.278	36.001	20.947	1.00	0.00
ATOM	4840	CD	PRO	A	612	39.221	37.125	21.071	1.00	0.00
ATOM	4841	CA	PRO	A	612	37.333	36.245	19.855	1.00	0.00
ATOM	4842	CB	PRO	A	612	37.844	37.554	19.247	1.00	0.00
ATOM	4843	CG	PRO	A	612	38.459	38.245	20.412	1.00	0.00
ATOM	4844	C	PRO	A	612	37.291	35.118	18.825	1.00	0.00
ATOM	4845	O	PRO	A	612	36.255	34.862	18.209	1.00	0.00
ATOM	4846	N	TYR	A	613	38.420	34.442	18.653	1.00	0.00
ATOM	4847	CA	TYR	A	613	38.528	33.373	17.669	1.00	0.00
ATOM	4848	CB	TYR	A	613	39.844	33.552	16.901	1.00	0.00
ATOM	4849	CG	TYR	A	613	41.068	33.594	17.795	1.00	0.00
ATOM	4850	CD1	TYR	A	613	41.675	32.421	18.235	1.00	0.00
ATOM	4851	CE1	TYR	A	613	42.776	32.455	19.089	1.00	0.00
ATOM	4852	CD2	TYR	A	613	41.598	34.813	18.235	1.00	0.00
ATOM	4853	CE2	TYR	A	613	42.699	34.854	19.094	1.00	0.00
ATOM	4854	CZ	TYR	A	613	43.278	33.675	19.514	1.00	0.00
ATOM	4855	OH	TYR	A	613	44.363	33.704	20.359	1.00	0.00
ATOM	4856	C	TYR	A	613	38.445	31.953	18.236	1.00	0.00
ATOM	4857	O	TYR	A	613	38.587	30.980	17.498	1.00	0.00
ATOM	4858	N	ALA	A	614	38.212	31.832	19.538	1.00	0.00
ATOM	4859	CA	ALA	A	614	38.139	30.518	20.166	1.00	0.00
ATOM	4860	CB	ALA	A	614	37.862	30.665	21.656	1.00	0.00
ATOM	4861	C	ALA	A	614	37.072	29.638	19.520	1.00	0.00
ATOM	4862	O	ALA	A	614	37.177	28.408	19.535	1.00	0.00
ATOM	4863	N	ASP	A	615	36.050	30.273	18.949	1.00	0.00
ATOM	4864	CA	ASP	A	615	34.963	29.547	18.302	1.00	0.00
ATOM	4865	CB	ASP	A	615	33.613	30.080	18.805	1.00	0.00
ATOM	4866	CG	ASP	A	615	33.436	31.567	18.552	1.00	0.00
ATOM	4867	OD1	ASP	A	615	33.122	31.951	17.402	1.00	0.00
ATOM	4868	OD2	ASP	A	615	33.620	32.357	19.504	1.00	0.00

88/396

Figure 1A-88

ATOM	4869	C	ASP	A	615	35.026	29.596	16.769	1.00	0.00
ATOM	4870	O	ASP	A	615	34.341	30.393	16.128	1.00	0.00
ATOM	4871	N	GLN	A	616	35.861	28.727	16.203	1.00	0.00
ATOM	4872	CA	GLN	A	616	36.062	28.594	14.757	1.00	0.00
ATOM	4873	CB	GLN	A	616	36.069	29.956	14.053	1.00	0.00
ATOM	4874	CG	GLN	A	616	34.702	30.364	13.521	1.00	0.00
ATOM	4875	CD	GLN	A	616	34.732	31.664	12.735	1.00	0.00
ATOM	4876	OE1	GLN	A	616	33.680	32.218	12.387	1.00	0.00
ATOM	4877	NE2	GLN	A	616	35.940	32.155	12.441	1.00	0.00
ATOM	4878	C	GLN	A	616	37.384	27.898	14.513	1.00	0.00
ATOM	4879	O	GLN	A	616	37.933	27.939	13.415	1.00	0.00
ATOM	4880	N	SER	A	617	37.885	27.239	15.547	1.00	0.00
ATOM	4881	CA	SER	A	617	39.159	26.561	15.443	1.00	0.00
ATOM	4882	CB	SER	A	617	40.115	27.115	16.502	1.00	0.00
ATOM	4883	OG	SER	A	617	40.202	28.524	16.418	1.00	0.00
ATOM	4884	C	SER	A	617	39.092	25.045	15.574	1.00	0.00
ATOM	4885	O	SER	A	617	38.256	24.499	16.293	1.00	0.00
ATOM	4886	N	ILE	A	618	39.987	24.377	14.855	1.00	0.00
ATOM	4887	CA	ILE	A	618	40.102	22.931	14.902	1.00	0.00
ATOM	4888	CB	ILE	A	618	40.181	22.311	13.499	1.00	0.00
ATOM	4889	CG2	ILE	A	618	40.451	20.821	13.623	1.00	0.00
ATOM	4890	CG1	ILE	A	618	38.882	22.563	12.728	1.00	0.00
ATOM	4891	CD1	ILE	A	618	38.626	24.008	12.379	1.00	0.00
ATOM	4892	C	ILE	A	618	41.426	22.702	15.615	1.00	0.00
ATOM	4893	O	ILE	A	618	42.422	23.344	15.286	1.00	0.00
ATOM	4894	N	LYS	A	619	41.446	21.802	16.591	1.00	0.00
ATOM	4895	CA	LYS	A	619	42.669	21.541	17.345	1.00	0.00
ATOM	4896	CB	LYS	A	619	42.328	21.339	18.827	1.00	0.00
ATOM	4897	CG	LYS	A	619	42.063	22.635	19.583	1.00	0.00
ATOM	4898	CD	LYS	A	619	41.465	22.377	20.958	1.00	0.00
ATOM	4899	CE	LYS	A	619	40.025	21.875	20.853	1.00	0.00
ATOM	4900	NZ	LYS	A	619	39.126	22.856	20.169	1.00	0.00
ATOM	4901	C	LYS	A	619	43.511	20.367	16.840	1.00	0.00
ATOM	4902	O	LYS	A	619	43.020	19.497	16.120	1.00	0.00
ATOM	4903	N	VAL	A	620	44.788	20.381	17.229	1.00	0.00
ATOM	4904	CA	VAL	A	620	45.785	19.362	16.880	1.00	0.00
ATOM	4905	CB	VAL	A	620	46.271	19.524	15.421	1.00	0.00
ATOM	4906	CG1	VAL	A	620	45.174	19.141	14.450	1.00	0.00
ATOM	4907	CG2	VAL	A	620	46.688	20.954	15.176	1.00	0.00
ATOM	4908	C	VAL	A	620	46.986	19.559	17.822	1.00	0.00
ATOM	4909	O	VAL	A	620	47.017	20.538	18.571	1.00	0.00
ATOM	4910	N	ALA	A	621	47.972	18.660	17.799	1.00	0.00
ATOM	4911	CA	ALA	A	621	49.123	18.832	18.690	1.00	0.00
ATOM	4912	CB	ALA	A	621	48.830	18.167	20.039	1.00	0.00
ATOM	4913	C	ALA	A	621	50.525	18.416	18.193	1.00	0.00
ATOM	4914	O	ALA	A	621	50.751	18.154	17.010	1.00	0.00
ATOM	4915	N	ALA	A	622	51.446	18.387	19.156	1.00	0.00
ATOM	4916	CA	ALA	A	622	52.883	18.079	19.046	1.00	0.00
ATOM	4917	CB	ALA	A	622	53.406	18.314	17.635	1.00	0.00
ATOM	4918	C	ALA	A	622	53.311	19.206	19.971	1.00	0.00
ATOM	4919	O	ALA	A	622	53.255	19.064	21.191	1.00	0.00
ATOM	4920	N	ALA	A	623	53.712	20.340	19.413	1.00	0.00
ATOM	4921	CA	ALA	A	623	54.006	21.459	20.286	1.00	0.00
ATOM	4922	CB	ALA	A	623	55.203	22.274	19.774	1.00	0.00
ATOM	4923	C	ALA	A	623	52.712	22.280	20.274	1.00	0.00
ATOM	4924	O	ALA	A	623	52.737	23.501	20.291	1.00	0.00

89/396

Figure 1A-89

ATOM	4925	N	ALA	A	624	51.583	21.569	20.213	1.00	0.00
ATOM	4926	CA	ALA	A	624	50.232	22.162	20.208	1.00	0.00
ATOM	4927	CB	ALA	A	624	50.003	22.957	21.496	1.00	0.00
ATOM	4928	C	ALA	A	624	49.902	23.048	18.996	1.00	0.00
ATOM	4929	O	ALA	A	624	50.788	23.683	18.421	1.00	0.00
ATOM	4930	N	ALA	A	625	48.622	23.087	18.612	1.00	0.00
ATOM	4931	CA	ALA	A	625	48.181	23.896	17.472	1.00	0.00
ATOM	4932	CB	ALA	A	625	48.840	23.386	16.190	1.00	0.00
ATOM	4933	C	ALA	A	625	46.663	23.957	17.279	1.00	0.00
ATOM	4934	O	ALA	A	625	45.948	22.994	17.549	1.00	0.00
ATOM	4935	N	ALA	A	626	46.196	25.104	16.789	1.00	0.00
ATOM	4936	CA	ALA	A	626	44.780	25.356	16.517	1.00	0.00
ATOM	4937	CB	ALA	A	626	44.110	25.959	17.746	1.00	0.00
ATOM	4938	C	ALA	A	626	44.744	26.344	15.355	1.00	0.00
ATOM	4939	O	ALA	A	626	45.712	27.076	15.159	1.00	0.00
ATOM	4940	N	ALA	A	804	43.646	26.384	14.597	1.00	0.00
ATOM	4941	CA	ALA	A	804	43.580	27.297	13.454	1.00	0.00
ATOM	4942	CB	ALA	A	804	44.324	26.671	12.275	1.00	0.00
ATOM	4943	C	ALA	A	804	42.194	27.781	12.986	1.00	0.00
ATOM	4944	O	ALA	A	804	41.161	27.279	13.421	1.00	0.00
ATOM	4945	N	ALA	A	805	42.203	28.764	12.082	1.00	0.00
ATOM	4946	CA	ALA	A	805	40.993	29.354	11.498	1.00	0.00
ATOM	4947	CB	ALA	A	805	40.476	30.491	12.386	1.00	0.00
ATOM	4948	C	ALA	A	805	41.358	29.886	10.108	1.00	0.00
ATOM	4949	O	ALA	A	805	42.495	29.720	9.675	1.00	0.00
ATOM	4950	N	ALA	A	806	40.419	30.531	9.415	1.00	0.00
ATOM	4951	CA	ALA	A	806	40.704	31.046	8.074	1.00	0.00
ATOM	4952	CB	ALA	A	806	40.466	29.933	7.032	1.00	0.00
ATOM	4953	C	ALA	A	806	39.935	32.306	7.672	1.00	0.00
ATOM	4954	O	ALA	A	806	38.878	32.592	8.208	1.00	0.00
ATOM	4955	N	ALA	A	807	40.480	33.042	6.707	1.00	0.00
ATOM	4956	CA	ALA	A	807	39.883	34.276	6.205	1.00	0.00
ATOM	4957	CB	ALA	A	807	40.362	35.458	7.056	1.00	0.00
ATOM	4958	C	ALA	A	807	40.394	34.406	4.767	1.00	0.00
ATOM	4959	O	ALA	A	807	40.848	33.411	4.205	1.00	0.00
ATOM	4960	N	ALA	A	808	40.343	35.601	4.169	1.00	0.00
ATOM	4961	CA	ALA	A	808	40.852	35.777	2.798	1.00	0.00
ATOM	4962	CB	ALA	A	808	39.964	35.032	1.812	1.00	0.00
ATOM	4963	C	ALA	A	808	40.989	37.236	2.362	1.00	0.00
ATOM	4964	O	ALA	A	808	40.000	37.864	1.987	1.00	0.00
ATOM	4965	N	ALA	A	809	42.222	37.749	2.388	1.00	0.00
ATOM	4966	CA	ALA	A	809	42.549	39.137	2.020	1.00	0.00
ATOM	4967	CB	ALA	A	809	43.091	39.195	0.602	1.00	0.00
ATOM	4968	C	ALA	A	809	41.359	40.078	2.157	1.00	0.00
ATOM	4969	O	ALA	A	809	40.634	40.312	1.185	1.00	0.00
ATOM	4970	N	ALA	A	810	41.187	40.611	3.370	1.00	0.00
ATOM	4971	CA	ALA	A	810	40.095	41.511	3.747	1.00	0.00
ATOM	4972	CB	ALA	A	810	39.421	42.133	2.514	1.00	0.00
ATOM	4973	C	ALA	A	810	39.078	40.702	4.545	1.00	0.00
ATOM	4974	O	ALA	A	810	39.425	39.692	5.167	1.00	0.00
ATOM	4975	N	ALA	A	811	39.852	40.806	7.281	1.00	0.00
ATOM	4976	CA	ALA	A	811	40.322	39.589	7.919	1.00	0.00
ATOM	4977	CB	ALA	A	811	41.797	39.710	8.251	1.00	0.00
ATOM	4978	C	ALA	A	811	39.519	39.348	9.192	1.00	0.00
ATOM	4979	O	ALA	A	811	40.095	39.012	10.227	1.00	0.00
ATOM	4980	N	ALA	A	812	38.193	39.502	9.114	1.00	0.00

90/396

Figure 1A-90

ATOM	4981	CA	ALA	A	812	37.332	39.338	10.284	1.00	0.00
ATOM	4982	CB	ALA	A	812	36.343	40.465	10.329	1.00	0.00
ATOM	4983	C	ALA	A	812	36.594	38.021	10.486	1.00	0.00
ATOM	4984	O	ALA	A	812	35.850	37.889	11.454	1.00	0.00
ATOM	4985	N	ALA	A	813	36.778	37.072	9.574	1.00	0.00
ATOM	4986	CA	ALA	A	813	36.174	35.748	9.685	1.00	0.00
ATOM	4987	CB	ALA	A	813	34.842	35.808	10.437	1.00	0.00
ATOM	4988	C	ALA	A	813	35.982	35.058	8.353	1.00	0.00
ATOM	4989	O	ALA	A	813	36.458	35.540	7.331	1.00	0.00
ATOM	4990	N	ALA	A	814	35.294	33.915	8.402	1.00	0.00
ATOM	4991	CA	ALA	A	814	34.985	33.059	7.251	1.00	0.00
ATOM	4992	CB	ALA	A	814	36.243	32.758	6.453	1.00	0.00
ATOM	4993	C	ALA	A	814	34.380	31.759	7.774	1.00	0.00
ATOM	4994	O	ALA	A	814	35.115	30.871	8.222	1.00	0.00
ATOM	4995	N	ALA	A	816	33.048	31.671	7.696	1.00	0.00
ATOM	4996	CA	ALA	A	816	32.261	30.519	8.151	1.00	0.00
ATOM	4997	CB	ALA	A	816	31.379	30.008	7.018	1.00	0.00
ATOM	4998	C	ALA	A	816	33.087	29.379	8.732	1.00	0.00
ATOM	4999	O	ALA	A	816	33.967	28.829	8.070	1.00	0.00
ATOM	5000	N	ALA	A	817	32.779	29.039	9.981	1.00	0.00
ATOM	5001	CA	ALA	A	817	33.462	27.983	10.726	1.00	0.00
ATOM	5002	CB	ALA	A	817	32.946	27.957	12.160	1.00	0.00
ATOM	5003	C	ALA	A	817	33.289	26.611	10.093	1.00	0.00
ATOM	5004	O	ALA	A	817	33.178	26.489	8.875	1.00	0.00
ATOM	5005	N	ALA	A	818	33.262	25.580	10.937	1.00	0.00
ATOM	5006	CA	ALA	A	818	33.099	24.201	10.479	1.00	0.00
ATOM	5007	CB	ALA	A	818	31.628	23.923	10.139	1.00	0.00
ATOM	5008	C	ALA	A	818	33.979	23.946	9.261	1.00	0.00
ATOM	5009	O	ALA	A	818	35.175	23.679	9.404	1.00	0.00
ATOM	5010	N	ALA	A	819	33.382	24.039	8.072	1.00	0.00
ATOM	5011	CA	ALA	A	819	34.094	23.824	6.817	1.00	0.00
ATOM	5012	CB	ALA	A	819	34.633	25.144	6.287	1.00	0.00
ATOM	5013	C	ALA	A	819	35.230	22.830	7.006	1.00	0.00
ATOM	5014	O	ALA	A	819	36.348	23.044	6.539	1.00	0.00
ATOM	5015	N	ALA	A	820	34.930	21.751	7.723	1.00	0.00
ATOM	5016	CA	ALA	A	820	35.899	20.694	7.979	1.00	0.00
ATOM	5017	CB	ALA	A	820	35.620	20.031	9.327	1.00	0.00
ATOM	5018	C	ALA	A	820	35.726	19.692	6.847	1.00	0.00
ATOM	5019	O	ALA	A	820	36.635	18.925	6.529	1.00	0.00
ATOM	5020	N	ALA	A	821	34.544	19.720	6.240	1.00	0.00
ATOM	5021	CA	ALA	A	821	34.219	18.836	5.128	1.00	0.00
ATOM	5022	CB	ALA	A	821	32.719	18.891	4.835	1.00	0.00
ATOM	5023	C	ALA	A	821	35.015	19.263	3.898	1.00	0.00
ATOM	5024	O	ALA	A	821	35.435	18.427	3.093	1.00	0.00
ATOM	5025	N	ALA	A	822	35.210	20.571	3.754	1.00	0.00
ATOM	5026	CA	ALA	A	822	35.976	21.100	2.633	1.00	0.00
ATOM	5027	CB	ALA	A	822	35.818	22.614	2.552	1.00	0.00
ATOM	5028	C	ALA	A	822	37.434	20.727	2.873	1.00	0.00
ATOM	5029	O	ALA	A	822	38.244	20.695	1.946	1.00	0.00
ATOM	5030	N	ALA	A	823	37.751	20.438	4.132	1.00	0.00
ATOM	5031	CA	ALA	A	823	39.097	20.051	4.527	1.00	0.00
ATOM	5032	CB	ALA	A	823	39.278	20.242	6.025	1.00	0.00
ATOM	5033	C	ALA	A	823	39.338	18.596	4.155	1.00	0.00
ATOM	5034	O	ALA	A	823	38.480	18.018	3.456	1.00	0.00
ATOM	5035	OXT	ALA	A	823	40.383	18.049	4.563	1.00	0.00
ATOM	5036	CB	ALA	A	661	59.666	27.186	11.041	1.00	0.00

91/396

Figure 1A-91

ATOM	5037	C	ALA	A	661	58.469	25.654	9.448	1.00	0.00
ATOM	5038	O	ALA	A	661	57.373	26.047	9.048	1.00	0.00
ATOM	5039	N	ALA	A	661	59.695	24.735	11.439	1.00	0.00
ATOM	5040	CA	ALA	A	661	58.884	25.875	10.907	1.00	0.00
ATOM	5041	N	ALA	A	662	59.335	25.027	8.654	1.00	0.00
ATOM	5042	CA	ALA	A	662	59.013	24.770	7.254	1.00	0.00
ATOM	5043	CB	ALA	A	662	60.252	24.279	6.501	1.00	0.00
ATOM	5044	C	ALA	A	662	57.887	23.743	7.155	1.00	0.00
ATOM	5045	O	ALA	A	662	57.282	23.562	6.096	1.00	0.00
ATOM	5046	N	ALA	A	663	57.613	23.065	8.265	1.00	0.00
ATOM	5047	CA	ALA	A	663	56.544	22.071	8.309	1.00	0.00
ATOM	5048	CB	ALA	A	663	56.746	21.134	9.497	1.00	0.00
ATOM	5049	C	ALA	A	663	55.217	22.823	8.438	1.00	0.00
ATOM	5050	O	ALA	A	663	54.207	22.446	7.834	1.00	0.00
ATOM	5051	N	ALA	A	664	55.237	23.897	9.225	1.00	0.00
ATOM	5052	CA	ALA	A	664	54.056	24.728	9.427	1.00	0.00
ATOM	5053	CB	ALA	A	664	54.364	25.852	10.412	1.00	0.00
ATOM	5054	C	ALA	A	664	53.607	25.313	8.093	1.00	0.00
ATOM	5055	O	ALA	A	664	52.430	25.223	7.739	1.00	0.00
ATOM	5056	N	ALA	A	665	54.550	25.909	7.360	1.00	0.00
ATOM	5057	CA	ALA	A	665	54.256	26.511	6.058	1.00	0.00
ATOM	5058	CB	ALA	A	665	55.549	26.977	5.368	1.00	0.00
ATOM	5059	C	ALA	A	665	53.555	25.492	5.189	1.00	0.00
ATOM	5060	O	ALA	A	665	52.584	25.812	4.496	1.00	0.00
ATOM	5061	N	ALA	A	666	54.066	24.263	5.236	1.00	0.00
ATOM	5062	CA	ALA	A	666	53.517	23.153	4.471	1.00	0.00
ATOM	5063	CB	ALA	A	666	54.337	21.890	4.730	1.00	0.00
ATOM	5064	C	ALA	A	666	52.070	22.935	4.880	1.00	0.00
ATOM	5065	O	ALA	A	666	51.154	22.974	4.046	1.00	0.00
ATOM	5066	N	ALA	A	667	51.862	22.714	6.172	1.00	0.00
ATOM	5067	CA	ALA	A	667	50.513	22.498	6.675	1.00	0.00
ATOM	5068	CB	ALA	A	667	50.523	22.382	8.200	1.00	0.00
ATOM	5069	C	ALA	A	667	49.611	23.644	6.243	1.00	0.00
ATOM	5070	O	ALA	A	667	48.593	23.422	5.586	1.00	0.00
ATOM	5071	N	ALA	A	668	49.997	24.869	6.599	1.00	0.00
ATOM	5072	CA	ALA	A	668	49.210	26.050	6.262	1.00	0.00
ATOM	5073	CB	ALA	A	668	49.905	27.314	6.768	1.00	0.00
ATOM	5074	C	ALA	A	668	48.974	26.146	4.769	1.00	0.00
ATOM	5075	O	ALA	A	668	47.885	26.516	4.329	1.00	0.00
ATOM	5076	N	ALA	A	669	49.996	25.806	3.991	1.00	0.00
ATOM	5077	CA	ALA	A	669	49.889	25.862	2.538	1.00	0.00
ATOM	5078	CB	ALA	A	669	51.259	25.669	1.902	1.00	0.00
ATOM	5079	C	ALA	A	669	48.908	24.810	2.023	1.00	0.00
ATOM	5080	O	ALA	A	669	48.178	25.048	1.062	1.00	0.00
ATOM	5081	N	ALA	A	670	48.891	23.648	2.669	1.00	0.00
ATOM	5082	CA	ALA	A	670	47.987	22.569	2.269	1.00	0.00
ATOM	5083	CB	ALA	A	670	48.454	21.249	2.866	1.00	0.00
ATOM	5084	C	ALA	A	670	46.553	22.871	2.714	1.00	0.00
ATOM	5085	O	ALA	A	670	45.618	22.806	1.907	1.00	0.00
ATOM	5086	N	ALA	A	671	46.382	23.198	3.996	1.00	0.00
ATOM	5087	CA	ALA	A	671	45.061	23.523	4.528	1.00	0.00
ATOM	5088	CB	ALA	A	671	45.173	24.059	5.952	1.00	0.00
ATOM	5089	C	ALA	A	671	44.456	24.574	3.618	1.00	0.00
ATOM	5090	O	ALA	A	671	43.265	24.539	3.316	1.00	0.00
ATOM	5091	N	ALA	A	672	45.295	25.506	3.175	1.00	0.00
ATOM	5092	CA	ALA	A	672	44.861	26.567	2.279	1.00	0.00

Figure 1A-92

ATOM	5093	CB	ALA	A	672	46.002	27.535	2.029	1.00	0.00
ATOM	5094	C	ALA	A	672	44.399	25.948	0.967	1.00	0.00
ATOM	5095	O	ALA	A	672	43.412	26.385	0.376	1.00	0.00
ATOM	5096	N	ALA	A	673	45.128	24.930	0.511	1.00	0.00
ATOM	5097	CA	ALA	A	673	44.778	24.243	-0.727	1.00	0.00
ATOM	5098	CB	ALA	A	673	45.696	23.043	-0.946	1.00	0.00
ATOM	5099	C	ALA	A	673	43.332	23.785	-0.593	1.00	0.00
ATOM	5100	O	ALA	A	673	42.505	24.007	-1.483	1.00	0.00
ATOM	5101	N	ALA	A	674	43.030	23.163	0.542	1.00	0.00
ATOM	5102	CA	ALA	A	674	41.680	22.685	0.805	1.00	0.00
ATOM	5103	CB	ALA	A	674	41.607	22.066	2.190	1.00	0.00
ATOM	5104	C	ALA	A	674	40.681	23.833	0.689	1.00	0.00
ATOM	5105	O	ALA	A	674	39.610	23.676	0.103	1.00	0.00
ATOM	5106	N	ALA	A	675	41.034	24.990	1.237	1.00	0.00
ATOM	5107	CA	ALA	A	675	40.145	26.142	1.181	1.00	0.00
ATOM	5108	CB	ALA	A	675	40.811	27.359	1.813	1.00	0.00
ATOM	5109	C	ALA	A	675	39.767	26.438	-0.262	1.00	0.00
ATOM	5110	O	ALA	A	675	38.592	26.398	-0.620	1.00	0.00
ATOM	5111	N	ALA	A	676	40.769	26.730	-1.087	1.00	0.00
ATOM	5112	CA	ALA	A	676	40.532	27.029	-2.496	1.00	0.00
ATOM	5113	CB	ALA	A	676	41.858	27.289	-3.212	1.00	0.00
ATOM	5114	C	ALA	A	676	39.802	25.849	-3.135	1.00	0.00
ATOM	5115	O	ALA	A	676	39.113	26.006	-4.148	1.00	0.00
ATOM	5116	N	ALA	A	677	39.955	24.674	-2.525	1.00	0.00
ATOM	5117	CA	ALA	A	677	39.310	23.452	-3.005	1.00	0.00
ATOM	5118	CB	ALA	A	677	40.109	22.225	-2.555	1.00	0.00
ATOM	5119	C	ALA	A	677	37.865	23.358	-2.498	1.00	0.00
ATOM	5120	O	ALA	A	677	37.394	22.279	-2.121	1.00	0.00
ATOM	5121	N	ALA	A	678	37.179	24.501	-2.485	1.00	0.00
ATOM	5122	CA	ALA	A	678	35.790	24.585	-2.048	1.00	0.00
ATOM	5123	CB	ALA	A	678	35.680	25.390	-0.760	1.00	0.00
ATOM	5124	C	ALA	A	678	35.000	25.259	-3.157	1.00	0.00
ATOM	5125	O	ALA	A	678	33.960	25.857	-2.919	1.00	0.00
ATOM	5126	N	ALA	A	679	35.522	25.165	-4.373	1.00	0.00
ATOM	5127	CA	ALA	A	679	34.885	25.735	-5.556	1.00	0.00
ATOM	5128	CB	ALA	A	679	33.631	24.916	-5.921	1.00	0.00
ATOM	5129	C	ALA	A	679	34.521	27.213	-5.417	1.00	0.00
ATOM	5130	O	ALA	A	679	33.579	27.563	-4.705	1.00	0.00
ATOM	5131	N	ALA	A	680	35.277	28.062	-6.113	1.00	0.00
ATOM	5132	CA	ALA	A	680	35.067	29.512	-6.126	1.00	0.00
ATOM	5133	CB	ALA	A	680	34.510	29.990	-4.785	1.00	0.00
ATOM	5134	C	ALA	A	680	36.365	30.257	-6.445	1.00	0.00
ATOM	5135	O	ALA	A	680	37.452	29.674	-6.425	1.00	0.00
ATOM	5136	N	ALA	A	686	36.243	31.550	-6.739	1.00	0.00
ATOM	5137	CA	ALA	A	686	37.400	32.387	-7.056	1.00	0.00
ATOM	5138	CB	ALA	A	686	36.935	33.702	-7.698	1.00	0.00
ATOM	5139	C	ALA	A	686	38.243	32.683	-5.812	1.00	0.00
ATOM	5140	O	ALA	A	686	39.345	33.225	-5.918	1.00	0.00
ATOM	5141	N	ALA	A	687	37.723	32.321	-4.641	1.00	0.00
ATOM	5142	CA	ALA	A	687	38.414	32.549	-3.369	1.00	0.00
ATOM	5143	CB	ALA	A	687	37.574	31.993	-2.208	1.00	0.00
ATOM	5144	C	ALA	A	687	39.825	31.947	-3.337	1.00	0.00
ATOM	5145	O	ALA	A	687	39.996	30.735	-3.188	1.00	0.00
ATOM	5146	N	ALA	A	688	40.828	32.814	-3.457	1.00	0.00
ATOM	5147	CA	ALA	A	688	42.226	32.397	-3.460	1.00	0.00
ATOM	5148	CB	ALA	A	688	43.016	33.293	-4.412	1.00	0.00

Figure 1A-93

ATOM	5149	C	ALA	A	688	42.881	32.396	-2.068	1.00	0.00
ATOM	5150	O	ALA	A	688	43.739	33.225	-1.778	1.00	0.00
ATOM	5151	N	ALA	A	689	42.482	31.456	-1.216	1.00	0.00
ATOM	5152	CA	ALA	A	689	43.043	31.354	0.127	1.00	0.00
ATOM	5153	CB	ALA	A	689	42.452	30.145	0.848	1.00	0.00
ATOM	5154	C	ALA	A	689	44.566	31.232	0.047	1.00	0.00
ATOM	5155	O	ALA	A	689	45.122	31.035	-1.037	1.00	0.00
ATOM	5156	N	ALA	A	690	45.240	31.346	1.189	1.00	0.00
ATOM	5157	CA	ALA	A	690	46.694	31.253	1.209	1.00	0.00
ATOM	5158	CB	ALA	A	690	47.286	32.538	0.693	1.00	0.00
ATOM	5159	C	ALA	A	690	47.248	30.939	2.595	1.00	0.00
ATOM	5160	O	ALA	A	690	46.533	31.007	3.589	1.00	0.00
ATOM	5161	N	ALA	A	691	48.524	30.585	2.652	1.00	0.00
ATOM	5162	CA	ALA	A	691	49.172	30.250	3.916	1.00	0.00
ATOM	5163	CB	ALA	A	691	50.676	30.029	3.689	1.00	0.00
ATOM	5164	C	ALA	A	691	48.956	31.347	4.960	1.00	0.00
ATOM	5165	O	ALA	A	691	48.705	31.071	6.138	1.00	0.00
ATOM	5166	N	ALA	A	692	49.057	32.592	4.511	1.00	0.00
ATOM	5167	CA	ALA	A	692	48.886	33.746	5.383	1.00	0.00
ATOM	5168	CB	ALA	A	692	49.425	35.010	4.695	1.00	0.00
ATOM	5169	C	ALA	A	692	47.426	33.936	5.771	1.00	0.00
ATOM	5170	O	ALA	A	692	47.119	34.658	6.717	1.00	0.00
ATOM	5171	N	ALA	A	693	46.525	33.286	5.044	1.00	0.00
ATOM	5172	CA	ALA	A	693	45.100	33.395	5.343	1.00	0.00
ATOM	5173	CB	ALA	A	693	44.288	33.390	4.055	1.00	0.00
ATOM	5174	C	ALA	A	693	44.648	32.263	6.271	1.00	0.00
ATOM	5175	O	ALA	A	693	43.459	32.102	6.530	1.00	0.00
ATOM	5176	N	ALA	A	694	45.608	31.485	6.767	1.00	0.00
ATOM	5177	CA	ALA	A	694	45.336	30.379	7.690	1.00	0.00
ATOM	5178	CB	ALA	A	694	45.831	29.040	7.094	1.00	0.00
ATOM	5179	C	ALA	A	694	46.085	30.700	8.979	1.00	0.00
ATOM	5180	O	ALA	A	694	47.305	30.581	9.038	1.00	0.00
ATOM	5181	N	ALA	A	695	45.348	31.098	10.012	1.00	0.00
ATOM	5182	CA	ALA	A	695	45.940	31.500	11.289	1.00	0.00
ATOM	5183	CB	ALA	A	695	45.176	32.718	11.829	1.00	0.00
ATOM	5184	C	ALA	A	695	46.043	30.433	12.377	1.00	0.00
ATOM	5185	O	ALA	A	695	45.034	29.949	12.880	1.00	0.00
ATOM	5186	N	ALA	A	696	47.275	30.099	12.755	1.00	0.00
ATOM	5187	CA	ALA	A	696	47.545	29.101	13.790	1.00	0.00
ATOM	5188	CB	ALA	A	696	48.773	28.269	13.405	1.00	0.00
ATOM	5189	C	ALA	A	696	47.759	29.756	15.155	1.00	0.00
ATOM	5190	O	ALA	A	696	48.389	30.807	15.252	1.00	0.00
ATOM	5191	N	ALA	A	697	47.230	29.126	16.202	1.00	0.00
ATOM	5192	CA	ALA	A	697	47.345	29.646	17.563	1.00	0.00
ATOM	5193	CB	ALA	A	697	46.005	30.212	18.020	1.00	0.00
ATOM	5194	C	ALA	A	697	47.813	28.563	18.536	1.00	0.00
ATOM	5195	O	ALA	A	697	47.988	27.401	18.149	1.00	0.00
ATOM	5196	N	ALA	A	698	47.999	28.944	19.800	1.00	0.00
ATOM	5197	CA	ALA	A	698	48.463	28.017	20.840	1.00	0.00
ATOM	5198	CB	ALA	A	698	47.559	26.793	20.911	1.00	0.00
ATOM	5199	C	ALA	A	698	49.911	27.612	20.530	1.00	0.00
ATOM	5200	O	ALA	A	698	50.753	28.479	20.285	1.00	0.00
ATOM	5201	N	ALA	A	699	50.209	26.317	20.533	1.00	0.00
ATOM	5202	CA	ALA	A	699	51.561	25.842	20.228	1.00	0.00
ATOM	5203	CB	ALA	A	699	51.977	26.317	18.830	1.00	0.00
ATOM	5204	C	ALA	A	699	52.646	26.230	21.249	1.00	0.00

Figure 1A-94

ATOM	5205	O	ALA	A	699	52.376	27.027	22.177	1.00	0.00
ATOM	5206	OXT	ALA	A	699	53.782	25.738	21.099	1.00	0.00
ATOM	5207	CB	ALA	A	701	54.820	10.723	15.170	1.00	0.00
ATOM	5208	C	ALA	A	701	53.011	12.130	16.177	1.00	0.00
ATOM	5209	O	ALA	A	701	53.725	13.099	15.911	1.00	0.00
ATOM	5210	N	ALA	A	701	52.456	10.240	14.647	1.00	0.00
ATOM	5211	CA	ALA	A	701	53.392	10.728	15.702	1.00	0.00
ATOM	5212	N	ALA	A	702	51.886	12.216	16.888	1.00	0.00
ATOM	5213	CA	ALA	A	702	51.348	13.466	17.438	1.00	0.00
ATOM	5214	CB	ALA	A	702	52.479	14.395	17.903	1.00	0.00
ATOM	5215	C	ALA	A	702	50.449	14.191	16.433	1.00	0.00
ATOM	5216	O	ALA	A	702	50.313	13.763	15.285	1.00	0.00
ATOM	5217	N	ALA	A	703	49.831	15.282	16.883	1.00	0.00
ATOM	5218	CA	ALA	A	703	48.918	16.102	16.074	1.00	0.00
ATOM	5219	CB	ALA	A	703	49.526	16.372	14.698	1.00	0.00
ATOM	5220	C	ALA	A	703	47.516	15.494	15.935	1.00	0.00
ATOM	5221	O	ALA	A	703	46.764	15.436	16.900	1.00	0.00
ATOM	5222	N	ALA	A	704	47.166	15.057	14.730	1.00	0.00
ATOM	5223	CA	ALA	A	704	45.861	14.438	14.465	1.00	0.00
ATOM	5224	CB	ALA	A	704	45.508	13.461	15.588	1.00	0.00
ATOM	5225	C	ALA	A	704	44.714	15.463	14.268	1.00	0.00
ATOM	5226	O	ALA	A	704	44.599	16.452	14.997	1.00	0.00
ATOM	5227	N	ALA	A	705	43.861	15.186	13.279	1.00	0.00
ATOM	5228	CA	ALA	A	705	42.722	16.025	12.867	1.00	0.00
ATOM	5229	CB	ALA	A	705	41.902	15.283	11.800	1.00	0.00
ATOM	5230	C	ALA	A	705	41.779	16.555	13.945	1.00	0.00
ATOM	5231	O	ALA	A	705	42.113	16.439	15.138	1.00	0.00
ATOM	5232	OXT	ALA	A	705	40.706	17.105	13.584	1.00	0.00
TER										
ATOM	5233	OH2	TIP	S	1	49.545	45.322	21.437	1.00	0.00
ATOM	5234	OH2	TIP	S	2	46.430	59.242	7.263	1.00	0.00
ATOM	5235	OH2	TIP	S	3	45.576	47.117	26.121	1.00	0.00
ATOM	5236	OH2	TIP	S	4	53.476	43.446	15.548	1.00	0.00
ATOM	5237	OH2	TIP	S	5	39.174	66.723	40.345	1.00	0.00
ATOM	5238	OH2	TIP	S	6	57.397	64.704	34.702	1.00	0.00
ATOM	5239	OH2	TIP	S	7	49.118	35.268	20.766	1.00	0.00
ATOM	5240	OH2	TIP	S	8	38.449	72.836	48.687	1.00	0.00
ATOM	5241	OH2	TIP	S	9	65.177	44.872	33.810	1.00	0.00
ATOM	5242	OH2	TIP	S	10	61.734	51.551	33.715	1.00	0.00
ATOM	5243	OH2	TIP	S	11	44.164	48.376	28.154	1.00	0.00
ATOM	5244	OH2	TIP	S	12	52.074	57.442	18.699	1.00	0.00
ATOM	5245	OH2	TIP	S	13	46.785	57.036	23.083	1.00	0.00
ATOM	5246	OH2	TIP	S	14	67.706	76.390	33.214	1.00	0.00
ATOM	5247	OH2	TIP	S	15	62.454	54.498	34.604	1.00	0.00
ATOM	5248	OH2	TIP	S	16	65.272	76.797	36.314	1.00	0.00
ATOM	5249	OH2	TIP	S	17	39.439	36.009	27.893	1.00	0.00
ATOM	5250	OH2	TIP	S	18	50.040	55.390	30.125	1.00	0.00
ATOM	5251	OH2	TIP	S	19	64.046	56.191	33.054	1.00	0.00
ATOM	5252	OH2	TIP	S	20	54.043	69.195	29.050	1.00	0.00
ATOM	5253	OH2	TIP	S	21	40.753	55.764	24.327	1.00	0.00
ATOM	5254	OH2	TIP	S	22	58.549	57.533	15.451	1.00	0.00
ATOM	5255	OH2	TIP	S	23	60.253	65.381	36.455	1.00	0.00
ATOM	5256	OH2	TIP	S	24	61.698	50.224	24.078	1.00	0.00
ATOM	5257	OH2	TIP	S	25	61.613	47.466	6.953	1.00	0.00
ATOM	5258	OH2	TIP	S	26	39.064	68.331	38.385	1.00	0.00
ATOM	5259	OH2	TIP	S	27	48.412	57.903	45.042	1.00	0.00

Figure 1A-95

ATOM	5260	OH2	TIP	S	28	60.806	42.181	36.580	1.00	0.00
ATOM	5261	OH2	TIP	S	29	51.139	59.951	50.711	1.00	0.00
ATOM	5262	OH2	TIP	S	30	45.463	55.515	18.760	1.00	0.00
ATOM	5263	OH2	TIP	S	31	62.718	73.493	50.939	1.00	0.00
ATOM	5264	OH2	TIP	S	32	45.978	46.445	21.875	1.00	0.00
ATOM	5265	OH2	TIP	S	33	72.481	42.488	29.968	1.00	0.00
ATOM	5266	OH2	TIP	S	34	36.393	42.674	35.604	1.00	0.00
ATOM	5267	OH2	TIP	S	35	52.413	74.700	55.230	1.00	0.00
ATOM	5268	OH2	TIP	S	36	67.542	43.906	36.141	1.00	0.00
ATOM	5269	OH2	TIP	S	37	49.414	57.114	23.258	1.00	0.00
ATOM	5270	OH2	TIP	S	38	37.080	62.007	45.468	1.00	0.00
ATOM	5271	OH2	TIP	S	39	29.740	41.211	41.369	1.00	0.00
ATOM	5272	OH2	TIP	S	40	51.029	43.063	41.914	1.00	0.00
ATOM	5273	OH2	TIP	S	41	43.298	56.630	18.617	1.00	0.00
ATOM	5274	OH2	TIP	S	42	49.385	62.046	50.513	1.00	0.00
ATOM	5275	OH2	TIP	S	43	63.737	57.222	28.504	1.00	0.00
ATOM	5276	OH2	TIP	S	44	66.689	61.391	43.589	1.00	0.00
ATOM	5277	OH2	TIP	S	45	45.233	43.402	37.391	1.00	0.00
ATOM	5278	OH2	TIP	S	46	57.633	79.130	41.470	1.00	0.00
ATOM	5279	OH2	TIP	S	47	41.624	49.507	20.692	1.00	0.00
ATOM	5280	OH2	TIP	S	48	31.085	62.069	24.688	1.00	0.00
ATOM	5281	OH2	TIP	S	49	56.072	49.126	49.409	1.00	0.00
ATOM	5282	OH2	TIP	S	50	52.128	89.974	43.293	1.00	0.00
ATOM	5283	OH2	TIP	S	51	58.050	55.804	42.785	1.00	0.00
ATOM	5284	OH2	TIP	S	52	27.159	50.867	25.633	1.00	0.00
ATOM	5285	OH2	TIP	S	53	65.256	66.995	45.459	1.00	0.00
ATOM	5286	OH2	TIP	S	54	77.914	73.472	41.334	1.00	0.00
ATOM	5287	OH2	TIP	S	55	32.437	67.370	39.272	1.00	0.00
ATOM	5288	OH2	TIP	S	56	63.024	46.701	48.192	1.00	0.00
ATOM	5289	OH2	TIP	S	57	58.950	40.116	11.627	1.00	0.00
ATOM	5290	OH2	TIP	S	58	50.939	64.827	32.040	1.00	0.00
ATOM	5291	OH2	TIP	S	59	70.989	83.801	40.551	1.00	0.00
ATOM	5292	OH2	TIP	S	60	57.886	33.984	32.530	1.00	0.00
ATOM	5293	OH2	TIP	S	61	79.175	83.227	24.694	1.00	0.00
ATOM	5294	OH2	TIP	S	62	72.082	57.977	14.047	1.00	0.00
ATOM	5295	OH2	TIP	S	63	73.538	42.017	25.376	1.00	0.00
ATOM	5296	OH2	TIP	S	64	47.388	39.741	9.561	1.00	0.00
ATOM	5297	OH2	TIP	S	65	35.330	48.191	0.775	1.00	0.00
ATOM	5298	OH2	TIP	S	66	69.794	46.455	40.493	1.00	0.00
ATOM	5299	OH2	TIP	S	67	57.631	83.285	34.350	1.00	0.00
ATOM	5300	OH2	TIP	S	68	52.038	62.712	30.807	1.00	0.00
ATOM	5301	OH2	TIP	S	69	43.073	85.517	22.282	1.00	0.00
ATOM	5302	OH2	TIP	S	70	62.355	45.818	9.059	1.00	0.00
ATOM	5303	OH2	TIP	S	71	40.439	57.423	9.123	1.00	0.00
ATOM	5304	OH2	TIP	S	72	65.467	56.496	26.919	1.00	0.00
ATOM	5305	OH2	TIP	S	73	86.710	72.670	26.417	1.00	0.00
ATOM	5306	OH2	TIP	S	74	62.405	88.458	33.079	1.00	0.00
ATOM	5307	OH2	TIP	S	75	68.838	73.543	48.200	1.00	0.00
ATOM	5308	OH2	TIP	S	76	29.142	41.201	23.270	1.00	0.00
ATOM	5309	OH2	TIP	S	77	52.651	30.829	11.843	1.00	0.00
ATOM	5310	OH2	TIP	S	78	38.003	52.214	6.763	1.00	0.00
ATOM	5311	OH2	TIP	S	79	76.403	64.571	23.916	1.00	0.00
ATOM	5312	OH2	TIP	S	80	43.479	61.575	15.985	1.00	0.00
ATOM	5313	OH2	TIP	S	81	53.654	48.191	4.663	1.00	0.00
ATOM	5314	OH2	TIP	S	82	31.209	38.380	40.229	1.00	0.00
ATOM	5315	OH2	TIP	S	83	51.898	83.417	38.956	1.00	0.00

96/396

Figure 1A-96

ATOM	5316	OH2	TIP	S	84	70.128	41.343	33.653	1.00	0.00
ATOM	5317	OH2	TIP	S	85	74.485	76.907	37.609	1.00	0.00
ATOM	5318	OH2	TIP	S	86	36.947	60.992	48.081	1.00	0.00
ATOM	5319	OH2	TIP	S	87	52.463	60.298	26.599	1.00	0.00
ATOM	5320	OH2	TIP	S	88	52.707	55.761	10.530	1.00	0.00
ATOM	5321	OH2	TIP	S	89	67.583	74.344	32.226	1.00	0.00
ATOM	5322	OH2	TIP	S	90	46.250	36.715	10.391	1.00	0.00
ATOM	5323	OH2	TIP	S	91	58.356	70.223	30.881	1.00	0.00
ATOM	5324	OH2	TIP	S	92	51.914	58.286	11.640	1.00	0.00
ATOM	5325	OH2	TIP	S	93	59.867	55.969	32.841	1.00	0.00
ATOM	5326	OH2	TIP	S	94	49.249	47.645	23.845	1.00	0.00
ATOM	5327	OH2	TIP	S	95	61.800	84.879	17.641	1.00	0.00
ATOM	5328	OH2	TIP	S	96	43.575	60.453	26.576	1.00	0.00
ATOM	5329	OH2	TIP	S	97	58.486	61.209	25.335	1.00	0.00
ATOM	5330	OH2	TIP	S	98	52.168	67.076	28.758	1.00	0.00
ATOM	5331	OH2	TIP	S	99	56.001	71.181	28.774	1.00	0.00
ATOM	5332	OH2	TIP	S	100	49.299	32.768	21.132	1.00	0.00
ATOM	5333	OH2	TIP	S	101	20.746	59.774	45.039	1.00	0.00
ATOM	5334	OH2	TIP	S	102	63.385	49.673	6.618	1.00	0.00
ATOM	5335	OH2	TIP	S	103	46.346	57.955	20.559	1.00	0.00
ATOM	5336	OH2	TIP	S	104	56.283	61.956	24.884	1.00	0.00
ATOM	5337	OH2	TIP	S	105	45.799	61.126	27.776	1.00	0.00
ATOM	5338	OH2	TIP	S	106	89.871	54.413	31.214	1.00	0.00
ATOM	5339	OH2	TIP	S	107	39.526	53.664	5.463	1.00	0.00
ATOM	5340	OH2	TIP	S	108	60.919	85.551	19.801	1.00	0.00
ATOM	5341	OH2	TIP	S	109	53.095	81.481	40.707	1.00	0.00
ATOM	5342	OH2	TIP	S	110	47.434	34.668	25.158	1.00	0.00
ATOM	5343	OH2	TIP	S	111	61.405	85.277	29.329	1.00	0.00
ATOM	5344	OH2	TIP	S	112	34.412	40.520	34.891	1.00	0.00
ATOM	5345	OH2	TIP	S	113	45.435	30.596	-3.577	1.00	0.00
ATOM	5346	OH2	TIP	S	114	62.179	69.082	43.392	1.00	0.00
ATOM	5347	OH2	TIP	S	115	61.044	48.007	48.516	1.00	0.00
ATOM	5348	OH2	TIP	S	116	28.016	74.646	28.335	1.00	0.00
ATOM	5349	OH2	TIP	S	117	67.037	59.393	42.026	1.00	0.00
ATOM	5350	OH2	TIP	S	118	101.749	64.917	50.857	1.00	0.00
ATOM	5351	OH2	TIP	S	119	47.038	35.531	12.699	1.00	0.00
ATOM	5352	OH2	TIP	S	120	46.432	59.634	23.553	1.00	0.00
ATOM	5353	OH2	TIP	S	121	70.309	58.874	15.612	1.00	0.00
ATOM	5354	OH2	TIP	S	122	63.948	54.921	18.151	1.00	0.00
ATOM	5355	OH2	TIP	S	123	23.442	50.302	29.826	1.00	0.00
ATOM	5356	OH2	TIP	S	124	70.237	49.693	43.253	1.00	0.00
ATOM	5357	OH2	TIP	S	125	63.252	79.627	44.372	1.00	0.00
ATOM	5358	OH2	TIP	S	126	69.591	61.709	44.302	1.00	0.00
ATOM	5359	OH2	TIP	S	127	74.744	75.727	21.968	1.00	0.00
ATOM	5360	OH2	TIP	S	128	67.375	79.057	15.093	1.00	0.00
ATOM	5361	OH2	TIP	S	129	28.201	37.666	43.253	1.00	0.00
ATOM	5362	OH2	TIP	S	130	46.238	63.550	31.339	1.00	0.00
ATOM	5363	OH2	TIP	S	131	70.323	40.312	30.964	1.00	0.00
ATOM	5364	OH2	TIP	S	132	27.856	77.993	33.358	1.00	0.00
ATOM	5365	OH2	TIP	S	133	82.160	46.121	17.111	1.00	0.00
ATOM	5366	OH2	TIP	S	134	85.327	58.267	38.423	1.00	0.00
ATOM	5367	OH2	TIP	S	135	62.797	35.947	15.959	1.00	0.00
ATOM	5368	OH2	TIP	S	136	70.557	51.932	47.024	1.00	0.00
ATOM	5369	OH2	TIP	S	137	41.834	79.830	37.050	1.00	0.00
ATOM	5370	OH2	TIP	S	138	25.075	57.946	43.494	1.00	0.00
ATOM	5371	OH2	TIP	S	139	49.849	60.012	52.953	1.00	0.00

97/396

Figure 1A-97

ATOM	5372	OH2	TIP	S	140	46.228	56.970	0.442	1.00	0.00
ATOM	5373	OH2	TIP	S	141	39.867	55.021	49.742	1.00	0.00
ATOM	5374	OH2	TIP	S	142	26.137	54.521	28.645	1.00	0.00
ATOM	5375	OH2	TIP	S	143	54.744	56.972	4.347	1.00	0.00
ATOM	5376	OH2	TIP	S	144	72.551	60.558	46.556	1.00	0.00
ATOM	5377	OH2	TIP	S	145	53.103	57.696	13.998	1.00	0.00
ATOM	5378	OH2	TIP	S	146	49.609	68.736	53.951	1.00	0.00
ATOM	5379	OH2	TIP	S	147	51.842	88.154	26.297	1.00	0.00
ATOM	5380	OH2	TIP	S	148	52.295	34.105	31.446	1.00	0.00
ATOM	5381	OH2	TIP	S	149	65.771	48.152	7.469	1.00	0.00
ATOM	5382	OH2	TIP	S	150	64.845	75.303	26.789	1.00	0.00
ATOM	5383	OH2	TIP	S	151	31.517	53.943	13.065	1.00	0.00
ATOM	5384	OH2	TIP	S	152	24.466	50.588	27.185	1.00	0.00
ATOM	5385	OH2	TIP	S	153	26.997	77.809	43.088	1.00	0.00
ATOM	5386	OH2	TIP	S	154	41.880	53.224	-6.568	1.00	0.00
ATOM	5387	OH2	TIP	S	155	34.987	24.863	13.451	1.00	0.00
ATOM	5388	OH2	TIP	S	156	39.707	16.302	1.430	1.00	0.00
ATOM	5389	OH2	TIP	S	157	58.133	62.698	23.192	1.00	0.00
ATOM	5390	OH2	TIP	S	158	64.974	46.487	9.154	1.00	0.00
ATOM	5391	OH2	TIP	S	159	30.468	25.555	-4.755	1.00	0.00
ATOM	5392	OH2	TIP	S	160	70.439	59.658	43.446	1.00	0.00
ATOM	5393	OH2	TIP	S	161	71.225	40.547	25.618	1.00	0.00
ATOM	5394	OH2	TIP	S	162	49.787	34.114	24.375	1.00	0.00
ATOM	5395	OH2	TIP	S	163	50.558	60.878	28.233	1.00	0.00
ATOM	5396	OH2	TIP	S	164	51.300	58.040	21.406	1.00	0.00
ATOM	5397	OH2	TIP	S	165	52.553	60.603	10.791	1.00	0.00
ATOM	5398	OH2	TIP	S	166	64.908	45.104	47.522	1.00	0.00
ATOM	5399	OH2	TIP	S	167	59.572	68.152	31.727	1.00	0.00
ATOM	5400	OH2	TIP	S	168	61.089	65.260	33.564	1.00	0.00
ATOM	5401	OH2	TIP	S	169	65.053	57.085	19.063	1.00	0.00
ATOM	5402	OH2	TIP	S	170	78.141	85.223	23.463	1.00	0.00
ATOM	5403	OH2	TIP	S	171	30.921	42.779	33.082	1.00	0.00
ATOM	5404	OH2	TIP	S	172	78.008	77.003	47.812	1.00	0.00
ATOM	5405	OH2	TIP	S	173	52.953	69.613	20.177	1.00	0.00
ATOM	5406	OH2	TIP	S	174	44.851	40.637	37.415	1.00	0.00
ATOM	5407	OH2	TIP	S	175	32.363	68.427	37.128	1.00	0.00
ATOM	5408	OH2	TIP	S	176	21.535	58.149	42.965	1.00	0.00
ATOM	5409	OH2	TIP	S	177	73.147	58.653	44.906	1.00	0.00
ATOM	5410	OH2	TIP	S	178	44.298	48.610	30.952	1.00	0.00
ATOM	5411	OH2	TIP	S	179	68.210	72.267	33.291	1.00	0.00
ATOM	5412	OH2	TIP	S	180	64.575	57.877	30.906	1.00	0.00
ATOM	5413	OH2	TIP	S	181	68.974	63.943	42.760	1.00	0.00
ATOM	5414	OH2	TIP	S	182	29.990	68.185	39.130	1.00	0.00
ATOM	5415	OH2	TIP	S	183	65.633	50.484	5.013	1.00	0.00
ATOM	5416	OH2	TIP	S	184	63.305	82.091	39.855	1.00	0.00
ATOM	5417	OH2	TIP	S	185	45.405	58.277	51.657	1.00	0.00
ATOM	5418	OH2	TIP	S	186	50.432	73.475	25.286	1.00	0.00
ATOM	5419	OH2	TIP	S	187	62.153	85.489	11.340	1.00	0.00
ATOM	5420	OH2	TIP	S	188	54.629	55.369	2.331	1.00	0.00
ATOM	5421	OH2	TIP	S	189	60.230	86.440	12.553	1.00	0.00
ATOM	5422	OH2	TIP	S	190	24.113	77.326	34.487	1.00	0.00
ATOM	5423	OH2	TIP	S	191	64.861	58.321	22.765	1.00	0.00
ATOM	5424	OH2	TIP	S	192	36.546	69.221	38.424	1.00	0.00
ATOM	5425	OH2	TIP	S	193	65.223	35.438	15.702	1.00	0.00
ATOM	5426	OH2	TIP	S	194	87.133	75.766	27.787	1.00	0.00
ATOM	5427	OH2	TIP	S	195	61.803	64.750	31.169	1.00	0.00

Figure 1A-98

ATOM	5428	OH2	TIP	S	196	50.015	31.115	0.565	1.00	0.00
ATOM	5429	OH2	TIP	S	197	47.825	58.968	3.834	1.00	0.00
ATOM	5430	OH2	TIP	S	198	77.648	78.449	49.907	1.00	0.00
ATOM	5431	OH2	TIP	S	199	56.545	62.003	27.647	1.00	0.00
ATOM	5432	OH2	TIP	S	200	60.906	36.243	14.318	1.00	0.00
ATOM	5433	OH2	TIP	S	201	41.818	82.799	38.633	1.00	0.00
ATOM	5434	OH2	TIP	S	202	59.264	34.150	30.565	1.00	0.00
ATOM	5435	OH2	TIP	S	203	66.928	61.068	39.278	1.00	0.00
ATOM	5436	OH2	TIP	S	204	34.771	60.324	49.396	1.00	0.00
ATOM	5437	OH2	TIP	S	205	63.471	86.821	30.804	1.00	0.00
ATOM	5438	OH2	TIP	S	206	80.068	80.750	40.682	1.00	0.00
ATOM	5439	OH2	TIP	S	207	41.388	49.118	44.350	1.00	0.00
ATOM	5440	OH2	TIP	S	208	40.133	68.846	42.367	1.00	0.00
ATOM	5441	OH2	TIP	S	209	35.025	51.167	21.015	1.00	0.00
ATOM	5442	OH2	TIP	S	210	20.825	50.960	29.294	1.00	0.00
ATOM	5443	OH2	TIP	S	211	88.602	74.058	25.989	1.00	0.00
ATOM	5444	OH2	TIP	S	212	70.173	39.513	28.574	1.00	0.00
ATOM	5445	OH2	TIP	S	213	56.207	68.585	55.519	1.00	0.00
ATOM	5446	OH2	TIP	S	214	58.580	53.605	44.475	1.00	0.00
ATOM	5447	OH2	TIP	S	215	71.181	80.846	19.234	1.00	0.00
ATOM	5448	OH2	TIP	S	216	71.298	54.679	22.333	1.00	0.00
ATOM	5449	OH2	TIP	S	217	51.078	66.793	54.324	1.00	0.00
ATOM	5450	OH2	TIP	S	218	82.401	46.359	20.147	1.00	0.00
ATOM	5451	OH2	TIP	S	219	66.873	70.741	51.833	1.00	0.00
ATOM	5452	OH2	TIP	S	220	84.553	72.308	33.318	1.00	0.00
ATOM	5453	OH2	TIP	S	221	39.989	74.333	50.382	1.00	0.00
ATOM	5454	OH2	TIP	S	222	74.830	77.654	12.721	1.00	0.00
ATOM	5455	OH2	TIP	S	223	80.634	47.015	22.774	1.00	0.00
ATOM	5456	OH2	TIP	S	224	47.118	34.445	30.617	1.00	0.00
ATOM	5457	OH2	TIP	S	225	22.888	50.661	24.553	1.00	0.00
ATOM	5458	OH2	TIP	S	226	42.927	83.463	21.069	1.00	0.00
ATOM	5459	OH2	TIP	S	227	48.316	46.525	4.414	1.00	0.00
ATOM	5460	OH2	TIP	S	228	49.891	62.644	8.759	1.00	0.00
ATOM	5461	OH2	TIP	S	229	29.803	62.508	22.532	1.00	0.00
ATOM	5462	OH2	TIP	S	230	28.084	73.736	31.489	1.00	0.00
ATOM	5463	OH2	TIP	S	231	78.563	55.242	33.677	1.00	0.00
ATOM	5464	OH2	TIP	S	232	63.452	82.015	43.955	1.00	0.00
ATOM	5465	OH2	TIP	S	233	75.583	59.672	56.212	1.00	0.00
ATOM	5466	OH2	TIP	S	234	52.028	8.566	12.691	1.00	0.00
ATOM	5467	OH2	TIP	S	235	64.200	64.536	36.560	1.00	0.00
ATOM	5468	OH2	TIP	S	236	37.303	24.008	-5.092	1.00	0.00
ATOM	5469	OH2	TIP	S	237	18.881	57.883	45.897	1.00	0.00
ATOM	5470	OH2	TIP	S	238	58.391	63.966	30.390	1.00	0.00
ATOM	5471	OH2	TIP	S	239	31.256	23.376	-3.784	1.00	0.00
ATOM	5472	OH2	TIP	S	240	41.686	17.351	0.602	1.00	0.00
ATOM	5473	OH2	TIP	S	241	37.123	17.345	-0.521	1.00	0.00
ATOM	5474	OH2	TIP	S	242	35.536	53.935	20.852	1.00	0.00
ATOM	5475	OH2	TIP	S	243	37.504	16.270	1.902	1.00	0.00
ATOM	5476	OH2	TIP	S	244	69.385	60.818	38.067	1.00	0.00
ATOM	5477	OH2	TIP	S	245	47.307	62.027	23.014	1.00	0.00
ATOM	5478	OH2	TIP	S	246	42.050	15.408	2.627	1.00	0.00
ATOM	5479	OH2	TIP	S	247	48.067	12.150	13.784	1.00	0.00
ATOM	5480	OH2	TIP	S	248	48.364	62.410	19.477	1.00	0.00
ATOM	5481	OH2	TIP	S	249	49.644	33.763	1.920	1.00	0.00
ATOM	5482	OH2	TIP	S	250	54.898	69.141	26.890	1.00	0.00
ATOM	5483	OH2	TIP	S	251	35.622	22.575	14.573	1.00	0.00

Figure 1A-99

ATOM	5484	OH2	TIP	S	252	25.781	51.062	22.964	1.00	0.00
ATOM	5485	OH2	TIP	S	253	53.368	6.536	14.256	1.00	0.00
ATOM	5486	OH2	TIP	S	254	52.852	60.377	22.624	1.00	0.00
ATOM	5487	OH2	TIP	S	255	49.326	9.726	13.407	1.00	0.00
ATOM	5488	OH2	TIP	S	256	64.444	70.461	52.484	1.00	0.00
ATOM	5489	OH2	TIP	S	257	47.623	58.682	52.777	1.00	0.00
ATOM	5490	OH2	TIP	S	258	41.603	66.741	42.944	1.00	0.00
ATOM	5491	OH2	TIP	S	259	48.367	69.616	19.858	1.00	0.00
ATOM	5492	OH2	TIP	S	260	65.385	59.312	20.423	1.00	0.00
ATOM	5493	OH2	TIP	S	261	34.135	71.975	43.600	1.00	0.00
ATOM	5494	OH2	TIP	S	262	46.723	60.718	32.507	1.00	0.00
ATOM	5495	OH2	TIP	S	263	21.337	56.927	45.177	1.00	0.00
ATOM	5496	OH2	TIP	S	264	25.096	78.526	32.481	1.00	0.00
ATOM	5497	OH2	TIP	S	265	53.993	57.943	0.761	1.00	0.00
ATOM	5498	OH2	TIP	S	266	64.107	73.044	33.762	1.00	0.00
ATOM	5499	OH2	TIP	S	267	85.896	73.929	31.006	1.00	0.00
ATOM	5500	OH2	TIP	S	268	50.017	65.147	28.265	1.00	0.00
ATOM	5501	OH2	TIP	S	269	41.255	61.504	50.187	1.00	0.00
ATOM	5502	OH2	TIP	S	270	71.021	40.127	35.596	1.00	0.00
ATOM	5503	OH2	TIP	S	271	81.445	77.849	48.324	1.00	0.00
ATOM	5504	OH2	TIP	S	272	34.256	69.676	29.012	1.00	0.00
ATOM	5505	OH2	TIP	S	273	44.834	45.672	4.994	1.00	0.00
ATOM	5506	OH2	TIP	S	274	63.360	28.723	24.638	1.00	0.00
ATOM	5507	OH2	TIP	S	275	67.132	56.904	21.670	1.00	0.00
ATOM	5508	OH2	TIP	S	276	22.968	59.974	46.283	1.00	0.00
ATOM	5509	OH2	TIP	S	277	58.358	40.680	40.895	1.00	0.00
ATOM	5510	OH2	TIP	S	278	85.217	56.091	37.286	1.00	0.00
ATOM	5511	OH2	TIP	S	279	73.993	60.099	58.768	1.00	0.00
ATOM	5512	OH2	TIP	S	280	74.504	77.468	15.386	1.00	0.00
ATOM	5513	OH2	TIP	S	281	89.910	55.916	29.305	1.00	0.00
ATOM	5514	OH2	TIP	S	282	27.125	38.549	40.463	1.00	0.00
ATOM	5515	OH2	TIP	S	283	37.695	74.917	52.985	1.00	0.00
ATOM	5516	OH2	TIP	S	284	47.094	32.572	28.243	1.00	0.00
ATOM	5517	OH2	TIP	S	285	91.841	56.522	31.166	1.00	0.00
ATOM	5518	OH2	TIP	S	286	49.743	58.098	31.149	1.00	0.00
ATOM	5519	OH2	TIP	S	287	61.501	83.053	41.363	1.00	0.00
ATOM	5520	OH2	TIP	S	288	52.321	18.518	23.497	1.00	0.00
ATOM	5521	OH2	TIP	S	289	78.790	45.173	34.820	1.00	0.00
ATOM	5522	OH2	TIP	S	290	28.133	75.498	40.052	1.00	0.00
ATOM	5523	OH2	TIP	S	291	74.767	38.066	27.872	1.00	0.00
ATOM	5524	OH2	TIP	S	292	45.180	66.605	35.838	1.00	0.00
ATOM	5525	OH2	TIP	S	293	91.680	69.354	38.601	1.00	0.00
ATOM	5526	OH2	TIP	S	294	28.082	41.729	32.923	1.00	0.00
ATOM	5527	OH2	TIP	S	295	73.741	80.400	18.356	1.00	0.00
ATOM	5528	OH2	TIP	S	296	32.076	32.496	5.281	1.00	0.00
ATOM	5529	OH2	TIP	S	297	91.907	54.059	29.342	1.00	0.00
ATOM	5530	OH2	TIP	S	298	64.727	54.193	7.345	1.00	0.00
TER										
ATOM	5531	C1	NAG	N	800	78.925	71.175	49.271	1.00	0.00
ATOM	5532	C2	NAG	N	800	78.492	71.598	50.693	1.00	0.00
ATOM	5533	N2	NAG	N	800	77.567	70.609	51.219	1.00	0.00
ATOM	5534	C7	NAG	N	800	77.690	70.159	52.465	1.00	0.00
ATOM	5535	O7	NAG	N	800	78.362	69.168	52.756	1.00	0.00
ATOM	5536	C8	NAG	N	800	76.942	70.916	53.552	1.00	0.00
ATOM	5537	C3	NAG	N	800	77.814	72.983	50.698	1.00	0.00
ATOM	5538	O3	NAG	N	800	77.632	73.431	52.033	1.00	0.00

Figure 1A-100

[illegible]

101/396

Figure 2A-1

	<u>Atom</u>	<u>Type</u>	<u>Resid</u>	<u>#</u>	<u>X</u>	<u>Y</u>	<u>Z</u>	<u>Occ</u>	<u>B</u>
ATOM	1	CB	SER A	19	94.076	71.208	44.896	1.00	101.54
ATOM	2	OG	SER A	19	92.871	71.591	45.534	1.00	102.67
ATOM	3	C	SER A	19	94.111	68.905	45.899	1.00	100.56
ATOM	4	O	SER A	19	94.565	67.868	45.413	1.00	100.46
ATOM	5	N	SER A	19	96.209	69.971	45.139	1.00	100.69
ATOM	6	CA	SER A	19	94.875	70.223	45.758	1.00	101.00
ATOM	7	N	THR A	20	92.957	68.950	46.565	1.00	100.20
ATOM	8	CA	THR A	20	92.134	67.755	46.776	1.00	99.31
ATOM	9	CB	THR A	20	91.314	67.856	48.092	1.00	99.08
ATOM	10	OG1	THR A	20	92.205	67.978	49.207	1.00	101.08
ATOM	11	CG2	THR A	20	90.450	66.615	48.289	1.00	98.69
ATOM	12	C	THR A	20	91.160	67.507	45.627	1.00	98.41
ATOM	13	O	THR A	20	90.572	68.447	45.084	1.00	98.31
ATOM	14	N	ILE A	21	90.994	66.235	45.268	1.00	97.54
ATOM	15	CA	ILE A	21	90.081	65.831	44.198	1.00	97.28
ATOM	16	CB	ILE A	21	90.237	64.325	43.858	1.00	97.77
ATOM	17	CG2	ILE A	21	91.635	64.057	43.324	1.00	97.31
ATOM	18	CG1	ILE A	21	89.942	63.460	45.093	1.00	98.45
ATOM	19	CD1	ILE A	21	90.936	63.600	46.244	1.00	98.67
ATOM	20	C	ILE A	21	88.630	66.096	44.607	1.00	96.01
ATOM	21	O	ILE A	21	87.714	65.381	44.209	1.00	96.05
ATOM	22	N	GLU A	22	88.448	67.134	45.416	1.00	95.01
ATOM	23	CA	GLU A	22	87.148	67.551	45.920	1.00	92.83
ATOM	24	CB	GLU A	22	87.090	67.363	47.440	1.00	94.99
ATOM	25	CG	GLU A	22	85.952	68.105	48.130	1.00	96.65
ATOM	26	CD	GLU A	22	84.637	67.368	48.035	1.00	98.32
ATOM	27	OE1	GLU A	22	84.317	66.881	46.931	1.00	100.29
ATOM	28	OE2	GLU A	22	83.923	67.280	49.060	1.00	97.82
ATOM	29	C	GLU A	22	87.004	69.027	45.593	1.00	91.06
ATOM	30	O	GLU A	22	86.023	69.451	44.984	1.00	91.68
ATOM	31	N	GLU A	23	88.000	69.806	46.003	1.00	88.35
ATOM	32	CA	GLU A	23	87.988	71.239	45.762	1.00	86.30
ATOM	33	CB	GLU A	23	88.992	71.955	46.673	1.00	87.82
ATOM	34	CG	GLU A	23	88.960	73.477	46.538	1.00	89.74
ATOM	35	CD	GLU A	23	87.634	74.086	46.984	1.00	91.19
ATOM	36	OE1	GLU A	23	87.273	75.167	46.469	1.00	92.94
ATOM	37	OE2	GLU A	23	86.959	73.494	47.856	1.00	90.34
ATOM	38	C	GLU A	23	88.315	71.527	44.308	1.00	82.89
ATOM	39	O	GLU A	23	88.020	72.607	43.802	1.00	81.44
ATOM	40	N	GLN A	24	88.941	70.571	43.635	1.00	80.74
ATOM	41	CA	GLN A	24	89.252	70.774	42.229	1.00	81.11
ATOM	42	CB	GLN A	24	90.527	70.014	41.830	1.00	83.66
ATOM	43	CG	GLN A	24	90.488	68.508	42.000	1.00	86.80
ATOM	44	CD	GLN A	24	91.859	67.873	41.805	1.00	89.43
ATOM	45	OE1	GLN A	24	92.514	68.074	40.777	1.00	89.57
ATOM	46	NE2	GLN A	24	92.299	67.102	42.795	1.00	89.26
ATOM	47	C	GLN A	24	88.028	70.313	41.428	1.00	78.37
ATOM	48	O	GLN A	24	87.741	70.833	40.352	1.00	75.56
ATOM	49	N	ALA A	25	87.297	69.350	41.983	1.00	76.32
ATOM	50	CA	ALA A	25	86.083	68.857	41.353	1.00	73.73
ATOM	51	CB	ALA A	25	85.558	67.626	42.082	1.00	73.34
ATOM	52	C	ALA A	25	85.102	70.007	41.498	1.00	73.11

102/396

Figure 2A-2

ATOM	53	O	ALA	A	25	84.249	70.234	40.635	1.00	72.98
ATOM	54	N	LYS	A	26	85.232	70.739	42.599	1.00	69.92
ATOM	55	CA	LYS	A	26	84.361	71.875	42.833	1.00	68.00
ATOM	56	CB	LYS	A	26	84.533	72.418	44.253	1.00	69.82
ATOM	57	CG	LYS	A	26	83.840	71.613	45.340	1.00	70.63
ATOM	58	CD	LYS	A	26	83.882	72.371	46.658	1.00	70.88
ATOM	59	CE	LYS	A	26	82.970	71.756	47.697	1.00	71.40
ATOM	60	NZ	LYS	A	26	82.816	72.649	48.876	1.00	71.56
ATOM	61	C	LYS	A	26	84.640	72.984	41.832	1.00	65.54
ATOM	62	O	LYS	A	26	83.719	73.686	41.411	1.00	66.04
ATOM	63	N	THR	A	27	85.902	73.154	41.449	1.00	62.79
ATOM	64	CA	THR	A	27	86.228	74.208	40.498	1.00	61.42
ATOM	65	CB	THR	A	27	87.718	74.641	40.578	1.00	62.55
ATOM	66	OG1	THR	A	27	88.560	73.562	40.171	1.00	65.29
ATOM	67	CG2	THR	A	27	88.076	75.053	42.005	1.00	63.38
ATOM	68	C	THR	A	27	85.893	73.745	39.089	1.00	58.61
ATOM	69	O	THR	A	27	85.542	74.556	38.233	1.00	58.19
ATOM	70	N	PHE	A	28	85.993	72.441	38.855	1.00	56.10
ATOM	71	CA	PHE	A	28	85.651	71.880	37.557	1.00	55.75
ATOM	72	CB	PHE	A	28	85.897	70.373	37.549	1.00	56.76
ATOM	73	CG	PHE	A	28	85.161	69.643	36.455	1.00	61.93
ATOM	74	CD1	PHE	A	28	83.907	69.089	36.689	1.00	61.39
ATOM	75	CD2	PHE	A	28	85.719	69.516	35.187	1.00	63.07
ATOM	76	CE1	PHE	A	28	83.225	68.421	35.686	1.00	62.32
ATOM	77	CE2	PHE	A	28	85.038	68.846	34.171	1.00	64.34
ATOM	78	CZ	PHE	A	28	83.791	68.299	34.423	1.00	63.38
ATOM	79	C	PHE	A	28	84.171	72.165	37.298	1.00	54.30
ATOM	80	O	PHE	A	28	83.798	72.685	36.243	1.00	55.31
ATOM	81	N	LEU	A	29	83.344	71.837	38.285	1.00	52.36
ATOM	82	CA	LEU	A	29	81.907	72.048	38.221	1.00	53.48
ATOM	83	CB	LEU	A	29	81.240	71.472	39.473	1.00	52.64
ATOM	84	CG	LEU	A	29	80.455	70.159	39.384	1.00	54.98
ATOM	85	CD1	LEU	A	29	80.829	69.368	38.144	1.00	54.94
ATOM	86	CD2	LEU	A	29	80.713	69.356	40.649	1.00	55.28
ATOM	87	C	LEU	A	29	81.547	73.520	38.076	1.00	54.44
ATOM	88	O	LEU	A	29	80.617	73.869	37.347	1.00	55.44
ATOM	89	N	ASP	A	30	82.271	74.385	38.775	1.00	54.40
ATOM	90	CA	ASP	A	30	82.009	75.816	38.685	1.00	56.60
ATOM	91	CB	ASP	A	30	82.928	76.591	39.654	1.00	59.74
ATOM	92	CG	ASP	A	30	82.598	78.093	39.725	1.00	63.24
ATOM	93	OD1	ASP	A	30	81.407	78.464	39.821	1.00	65.85
ATOM	94	OD2	ASP	A	30	83.538	78.912	39.702	1.00	66.85
ATOM	95	C	ASP	A	30	82.231	76.272	37.233	1.00	54.01
ATOM	96	O	ASP	A	30	81.443	77.049	36.697	1.00	55.73
ATOM	97	N	LYS	A	31	83.292	75.785	36.597	1.00	51.61
ATOM	98	CA	LYS	A	31	83.572	76.156	35.211	1.00	55.03
ATOM	99	CB	LYS	A	31	84.928	75.593	34.766	1.00	56.11
ATOM	100	CG	LYS	A	31	86.122	76.173	35.526	1.00	61.08
ATOM	101	CD	LYS	A	31	87.450	75.664	34.969	1.00	63.16
ATOM	102	CE	LYS	A	31	88.626	76.120	35.835	1.00	65.01
ATOM	103	NZ	LYS	A	31	89.955	75.761	35.246	1.00	65.49
ATOM	104	C	LYS	A	31	82.452	75.652	34.279	1.00	54.62
ATOM	105	O	LYS	A	31	82.002	76.376	33.382	1.00	51.79
ATOM	106	N	PHE	A	32	82.013	74.414	34.512	1.00	51.60
ATOM	107	CA	PHE	A	32	80.941	73.785	33.746	1.00	50.26
ATOM	108	CB	PHE	A	32	80.681	72.373	34.285	1.00	51.61

103/396

Figure 2A-3

ATOM	109	CG	PHE	A	32	79.478	71.706	33.685	1.00	50.70
ATOM	110	CD1	PHE	A	32	78.218	71.859	34.262	1.00	49.40
ATOM	111	CD2	PHE	A	32	79.600	70.941	32.523	1.00	47.69
ATOM	112	CE1	PHE	A	32	77.094	71.256	33.683	1.00	48.67
ATOM	113	CE2	PHE	A	32	78.491	70.343	31.952	1.00	43.00
ATOM	114	CZ	PHE	A	32	77.239	70.500	32.529	1.00	43.83
ATOM	115	C	PHE	A	32	79.640	74.583	33.774	1.00	51.32
ATOM	116	O	PHE	A	32	79.073	74.909	32.732	1.00	51.21
ATOM	117	N	ASN	A	33	79.167	74.898	34.972	1.00	52.05
ATOM	118	CA	ASN	A	33	77.930	75.641	35.126	1.00	53.78
ATOM	119	CB	ASN	A	33	77.659	75.890	36.614	1.00	53.46
ATOM	120	CG	ASN	A	33	77.347	74.605	37.368	1.00	58.26
ATOM	121	OD1	ASN	A	33	77.387	74.564	38.593	1.00	63.74
ATOM	122	ND2	ASN	A	33	77.033	73.546	36.631	1.00	59.49
ATOM	123	C	ASN	A	33	77.907	76.947	34.339	1.00	55.01
ATOM	124	O	ASN	A	33	76.909	77.259	33.681	1.00	54.28
ATOM	125	N	HIS	A	34	79.000	77.705	34.389	1.00	56.91
ATOM	126	CA	HIS	A	34	79.058	78.965	33.654	1.00	53.40
ATOM	127	CB	HIS	A	34	80.243	79.809	34.129	1.00	51.86
ATOM	128	CG	HIS	A	34	80.052	80.381	35.499	1.00	50.04
ATOM	129	CD2	HIS	A	34	80.473	79.947	36.711	1.00	48.98
ATOM	130	ND1	HIS	A	34	79.236	81.468	35.744	1.00	50.49
ATOM	131	CE1	HIS	A	34	79.155	81.672	37.048	1.00	47.57
ATOM	132	NE2	HIS	A	34	79.894	80.760	37.657	1.00	48.27
ATOM	133	C	HIS	A	34	79.123	78.695	32.157	1.00	52.86
ATOM	134	O	HIS	A	34	78.407	79.326	31.388	1.00	55.39
ATOM	135	N	GLU	A	35	79.959	77.756	31.729	1.00	52.65
ATOM	136	CA	GLU	A	35	80.012	77.450	30.306	1.00	53.84
ATOM	137	CB	GLU	A	35	81.167	76.486	29.979	1.00	58.19
ATOM	138	CG	GLU	A	35	82.546	77.148	29.913	1.00	62.53
ATOM	139	CD	GLU	A	35	83.608	76.273	29.261	1.00	65.60
ATOM	140	OE1	GLU	A	35	83.793	75.122	29.710	1.00	68.00
ATOM	141	OE2	GLU	A	35	84.268	76.743	28.304	1.00	70.39
ATOM	142	C	GLU	A	35	78.690	76.837	29.836	1.00	53.13
ATOM	143	O	GLU	A	35	78.111	77.297	28.853	1.00	52.15
ATOM	144	N	ALA	A	36	78.210	75.817	30.554	1.00	52.45
ATOM	145	CA	ALA	A	36	76.965	75.117	30.206	1.00	51.03
ATOM	146	CB	ALA	A	36	76.672	73.985	31.211	1.00	47.96
ATOM	147	C	ALA	A	36	75.783	76.047	30.142	1.00	50.78
ATOM	148	O	ALA	A	36	74.994	75.982	29.210	1.00	50.92
ATOM	149	N	GLU	A	37	75.652	76.918	31.134	1.00	52.75
ATOM	150	CA	GLU	A	37	74.524	77.840	31.154	1.00	55.69
ATOM	151	CB	GLU	A	37	74.612	78.759	32.370	1.00	57.82
ATOM	152	CG	GLU	A	37	73.367	79.587	32.631	1.00	58.25
ATOM	153	CD	GLU	A	37	72.711	79.243	33.960	1.00	64.50
ATOM	154	OE1	GLU	A	37	73.401	78.669	34.843	1.00	65.20
ATOM	155	OE2	GLU	A	37	71.511	79.563	34.125	1.00	64.90
ATOM	156	C	GLU	A	37	74.479	78.684	29.882	1.00	56.88
ATOM	157	O	GLU	A	37	73.404	78.959	29.349	1.00	58.31
ATOM	158	N	ASP	A	38	75.648	79.101	29.401	1.00	58.56
ATOM	159	CA	ASP	A	38	75.717	79.921	28.192	1.00	59.55
ATOM	160	CB	ASP	A	38	77.087	80.595	28.081	1.00	61.75
ATOM	161	CG	ASP	A	38	77.252	81.355	26.781	1.00	64.97
ATOM	162	OD1	ASP	A	38	76.408	82.228	26.490	1.00	67.47
ATOM	163	OD2	ASP	A	38	78.227	81.075	26.049	1.00	67.02
ATOM	164	C	ASP	A	38	75.415	79.133	26.913	1.00	55.78

104/396

Figure 2A-4

ATOM	165	O	ASP	A	38	74.651	79.592	26.075	1.00	55.56
ATOM	166	N	LEU	A	39	75.998	77.950	26.765	1.00	52.45
ATOM	167	CA	LEU	A	39	75.742	77.151	25.570	1.00	54.43
ATOM	168	CB	LEU	A	39	76.720	75.979	25.478	1.00	54.53
ATOM	169	CG	LEU	A	39	78.152	76.349	25.108	1.00	57.93
ATOM	170	CD1	LEU	A	39	79.041	75.115	25.168	1.00	59.94
ATOM	171	CD2	LEU	A	39	78.167	76.952	23.704	1.00	59.92
ATOM	172	C	LEU	A	39	74.316	76.617	25.534	1.00	54.91
ATOM	173	O	LEU	A	39	73.726	76.466	24.458	1.00	57.10
ATOM	174	N	PHE	A	40	73.755	76.320	26.701	1.00	53.34
ATOM	175	CA	PHE	A	40	72.398	75.813	26.738	1.00	51.61
ATOM	176	CB	PHE	A	40	72.046	75.295	28.128	1.00	48.77
ATOM	177	CG	PHE	A	40	70.682	74.657	28.207	1.00	45.29
ATOM	178	CD1	PHE	A	40	70.486	73.348	27.768	1.00	48.36
ATOM	179	CD2	PHE	A	40	69.592	75.372	28.705	1.00	44.97
ATOM	180	CE1	PHE	A	40	69.221	72.754	27.821	1.00	47.91
ATOM	181	CE2	PHE	A	40	68.329	74.796	28.765	1.00	47.06
ATOM	182	CZ	PHE	A	40	68.141	73.482	28.321	1.00	47.95
ATOM	183	C	PHE	A	40	71.448	76.938	26.355	1.00	53.40
ATOM	184	O	PHE	A	40	70.425	76.704	25.708	1.00	53.95
ATOM	185	N	TYR	A	41	71.787	78.159	26.758	1.00	53.75
ATOM	186	CA	TYR	A	41	70.952	79.308	26.432	1.00	56.99
ATOM	187	CB	TYR	A	41	71.425	80.554	27.175	1.00	56.49
ATOM	188	CG	TYR	A	41	70.419	81.674	27.128	1.00	57.13
ATOM	189	CD1	TYR	A	41	69.202	81.560	27.786	1.00	57.98
ATOM	190	CE1	TYR	A	41	68.254	82.579	27.737	1.00	61.44
ATOM	191	CD2	TYR	A	41	70.671	82.843	26.411	1.00	60.62
ATOM	192	CE2	TYR	A	41	69.723	83.874	26.354	1.00	61.17
ATOM	193	CZ	TYR	A	41	68.516	83.732	27.021	1.00	62.36
ATOM	194	OH	TYR	A	41	67.560	84.728	26.969	1.00	64.01
ATOM	195	C	TYR	A	41	70.959	79.594	24.927	1.00	58.92
ATOM	196	O	TYR	A	41	69.923	79.927	24.347	1.00	58.47
ATOM	197	N	GLN	A	42	72.128	79.475	24.302	1.00	59.96
ATOM	198	CA	GLN	A	42	72.250	79.714	22.868	1.00	62.60
ATOM	199	CB	GLN	A	42	73.725	79.686	22.447	1.00	63.34
ATOM	200	CG	GLN	A	42	74.552	80.874	22.980	1.00	68.67
ATOM	201	CD	GLN	A	42	76.063	80.741	22.730	1.00	71.49
ATOM	202	OE1	GLN	A	42	76.516	80.571	21.593	1.00	74.48
ATOM	203	NE2	GLN	A	42	76.843	80.828	23.798	1.00	72.57
ATOM	204	C	GLN	A	42	71.463	78.636	22.125	1.00	64.02
ATOM	205	O	GLN	A	42	70.714	78.927	21.189	1.00	66.04
ATOM	206	N	SER	A	43	71.625	77.392	22.561	1.00	63.34
ATOM	207	CA	SER	A	43	70.928	76.269	21.960	1.00	61.32
ATOM	208	CB	SER	A	43	71.415	74.962	22.570	1.00	63.15
ATOM	209	OG	SER	A	43	70.759	73.863	21.975	1.00	62.80
ATOM	210	C	SER	A	43	69.424	76.385	22.156	1.00	62.60
ATOM	211	O	SER	A	43	68.654	76.047	21.250	1.00	64.28
ATOM	212	N	SER	A	44	69.004	76.858	23.331	1.00	59.50
ATOM	213	CA	SER	A	44	67.583	77.025	23.624	1.00	58.22
ATOM	214	CB	SER	A	44	67.369	77.376	25.101	1.00	60.77
ATOM	215	OG	SER	A	44	67.648	76.269	25.936	1.00	61.14
ATOM	216	C	SER	A	44	66.933	78.103	22.757	1.00	58.11
ATOM	217	O	SER	A	44	65.861	77.883	22.180	1.00	52.67
ATOM	218	N	LEU	A	45	67.577	79.269	22.694	1.00	58.39
ATOM	219	CA	LEU	A	45	67.088	80.397	21.898	1.00	61.00
ATOM	220	CB	LEU	A	45	68.042	81.582	21.999	1.00	63.63

105/396

Figure 2A-5

ATOM	221	CG	LEU	A	45	67.610	82.737	22.894	1.00	67.42
ATOM	222	CD1	LEU	A	45	68.811	83.627	23.191	1.00	68.91
ATOM	223	CD2	LEU	A	45	66.496	83.520	22.205	1.00	69.14
ATOM	224	C	LEU	A	45	66.950	80.002	20.438	1.00	60.25
ATOM	225	O	LEU	A	45	66.000	80.384	19.770	1.00	59.50
ATOM	226	N	ALA	A	46	67.913	79.239	19.945	1.00	60.50
ATOM	227	CA	ALA	A	46	67.869	78.785	18.569	1.00	60.74
ATOM	228	CB	ALA	A	46	69.116	77.983	18.244	1.00	61.94
ATOM	229	C	ALA	A	46	66.628	77.926	18.357	1.00	63.18
ATOM	230	O	ALA	A	46	65.857	78.170	17.431	1.00	65.59
ATOM	231	N	SER	A	47	66.438	76.919	19.212	1.00	63.01
ATOM	232	CA	SER	A	47	65.284	76.033	19.095	1.00	61.51
ATOM	233	CB	SER	A	47	65.335	74.924	20.146	1.00	60.98
ATOM	234	OG	SER	A	47	66.327	73.967	19.813	1.00	64.94
ATOM	235	C	SER	A	47	63.973	76.783	19.226	1.00	61.07
ATOM	236	O	SER	A	47	62.967	76.401	18.637	1.00	60.36
ATOM	237	N	TRP	A	48	63.983	77.855	20.000	1.00	61.61
ATOM	238	CA	TRP	A	48	62.778	78.635	20.195	1.00	63.89
ATOM	239	CB	TRP	A	48	62.972	79.601	21.361	1.00	65.65
ATOM	240	CG	TRP	A	48	61.871	80.583	21.495	1.00	68.44
ATOM	241	CD2	TRP	A	48	60.668	80.414	22.247	1.00	68.83
ATOM	242	CE2	TRP	A	48	59.891	81.580	22.058	1.00	68.99
ATOM	243	CE3	TRP	A	48	60.168	79.389	23.062	1.00	68.58
ATOM	244	CD1	TRP	A	48	61.785	81.808	20.895	1.00	69.02
ATOM	245	NE1	TRP	A	48	60.597	82.414	21.230	1.00	71.37
ATOM	246	CZ2	TRP	A	48	58.639	81.751	22.654	1.00	70.16
ATOM	247	CZ3	TRP	A	48	58.923	79.555	23.656	1.00	67.97
ATOM	248	CH2	TRP	A	48	58.171	80.730	23.448	1.00	69.94
ATOM	249	C	TRP	A	48	62.415	79.395	18.925	1.00	65.19
ATOM	250	O	TRP	A	48	61.243	79.578	18.622	1.00	65.60
ATOM	251	N	ASN	A	49	63.431	79.839	18.193	1.00	67.01
ATOM	252	CA	ASN	A	49	63.230	80.572	16.950	1.00	68.09
ATOM	253	CB	ASN	A	49	64.567	81.017	16.369	1.00	66.69
ATOM	254	CG	ASN	A	49	65.159	82.184	17.106	1.00	64.84
ATOM	255	OD1	ASN	A	49	66.355	82.452	16.996	1.00	67.13
ATOM	256	ND2	ASN	A	49	64.326	82.904	17.854	1.00	65.30
ATOM	257	C	ASN	A	49	62.546	79.665	15.954	1.00	69.92
ATOM	258	O	ASN	A	49	61.585	80.063	15.305	1.00	71.21
ATOM	259	N	TYR	A	50	63.053	78.440	15.849	1.00	70.16
ATOM	260	CA	TYR	A	50	62.520	77.441	14.931	1.00	71.98
ATOM	261	CB	TYR	A	50	63.460	76.240	14.887	1.00	74.19
ATOM	262	CG	TYR	A	50	62.905	75.051	14.141	1.00	78.56
ATOM	263	CD1	TYR	A	50	62.982	74.972	12.751	1.00	81.07
ATOM	264	CE1	TYR	A	50	62.485	73.865	12.066	1.00	81.61
ATOM	265	CD2	TYR	A	50	62.310	73.996	14.829	1.00	79.21
ATOM	266	CE2	TYR	A	50	61.810	72.889	14.157	1.00	81.11
ATOM	267	CZ	TYR	A	50	61.902	72.828	12.777	1.00	82.31
ATOM	268	OH	TYR	A	50	61.412	71.727	12.117	1.00	83.75
ATOM	269	C	TYR	A	50	61.100	76.953	15.238	1.00	73.03
ATOM	270	O	TYR	A	50	60.336	76.662	14.312	1.00	74.83
ATOM	271	N	ASN	A	51	60.745	76.847	16.519	1.00	70.91
ATOM	272	CA	ASN	A	51	59.407	76.383	16.887	1.00	70.54
ATOM	273	CB	ASN	A	51	59.407	75.703	18.266	1.00	66.35
ATOM	274	CG	ASN	A	51	60.060	74.334	18.243	1.00	62.82
ATOM	275	OD1	ASN	A	51	61.278	74.218	18.127	1.00	64.96
ATOM	276	ND2	ASN	A	51	59.248	73.286	18.343	1.00	60.30

106/396

Figure 2A-6

ATOM	277	C	ASN	A	51	58.388	77.510	16.891	1.00	72.69
ATOM	278	O	ASN	A	51	57.193	77.266	17.037	1.00	74.24
ATOM	279	N	THR	A	52	58.859	78.743	16.740	1.00	74.39
ATOM	280	CA	THR	A	52	57.974	79.905	16.716	1.00	76.14
ATOM	281	CB	THR	A	52	58.457	80.991	17.685	1.00	76.16
ATOM	282	OG1	THR	A	52	59.833	81.289	17.414	1.00	75.42
ATOM	283	CG2	THR	A	52	58.297	80.531	19.126	1.00	77.50
ATOM	284	C	THR	A	52	57.913	80.512	15.316	1.00	77.38
ATOM	285	O	THR	A	52	56.993	81.263	14.989	1.00	77.97
ATOM	286	N	ASN	A	53	58.914	80.186	14.505	1.00	79.14
ATOM	287	CA	ASN	A	53	59.014	80.673	13.138	1.00	78.73
ATOM	288	CB	ASN	A	53	59.807	81.977	13.068	1.00	81.12
ATOM	289	CG	ASN	A	53	59.976	82.476	11.637	1.00	83.83
ATOM	290	OD1	ASN	A	53	60.850	83.299	11.347	1.00	85.38
ATOM	291	ND2	ASN	A	53	59.131	81.982	10.736	1.00	83.38
ATOM	292	C	ASN	A	53	59.741	79.636	12.317	1.00	79.15
ATOM	293	O	ASN	A	53	60.932	79.782	12.046	1.00	76.94
ATOM	294	N	ILE	A	54	59.032	78.584	11.928	1.00	80.77
ATOM	295	CA	ILE	A	54	59.643	77.542	11.129	1.00	83.05
ATOM	296	CB	ILE	A	54	58.611	76.473	10.731	1.00	84.24
ATOM	297	CG2	ILE	A	54	59.276	75.391	9.891	1.00	84.90
ATOM	298	CG1	ILE	A	54	58.002	75.859	11.998	1.00	86.26
ATOM	299	CD1	ILE	A	54	57.053	74.686	11.751	1.00	85.53
ATOM	300	C	ILE	A	54	60.250	78.174	9.882	1.00	85.54
ATOM	301	O	ILE	A	54	59.548	78.779	9.068	1.00	86.47
ATOM	302	N	THR	A	55	61.568	78.048	9.763	1.00	87.52
ATOM	303	CA	THR	A	55	62.332	78.586	8.638	1.00	88.94
ATOM	304	CB	THR	A	55	62.987	79.951	9.011	1.00	88.64
ATOM	305	OG1	THR	A	55	61.994	80.988	8.991	1.00	87.61
ATOM	306	CG2	THR	A	55	64.094	80.306	8.047	1.00	87.56
ATOM	307	C	THR	A	55	63.419	77.565	8.299	1.00	90.88
ATOM	308	O	THR	A	55	63.707	76.672	9.100	1.00	92.00
ATOM	309	N	GLU	A	56	64.011	77.677	7.114	1.00	92.49
ATOM	310	CA	GLU	A	56	65.061	76.745	6.715	1.00	94.04
ATOM	311	CB	GLU	A	56	65.238	76.747	5.194	1.00	95.34
ATOM	312	CG	GLU	A	56	66.258	75.725	4.716	1.00	96.49
ATOM	313	CD	GLU	A	56	65.912	74.318	5.167	1.00	98.07
ATOM	314	OE1	GLU	A	56	66.770	73.415	5.018	1.00	98.43
ATOM	315	OE2	GLU	A	56	64.780	74.117	5.666	1.00	97.44
ATOM	316	C	GLU	A	56	66.395	77.078	7.388	1.00	94.03
ATOM	317	O	GLU	A	56	67.187	76.185	7.698	1.00	93.34
ATOM	318	N	GLU	A	57	66.647	78.366	7.601	1.00	92.92
ATOM	319	CA	GLU	A	57	67.878	78.779	8.252	1.00	92.81
ATOM	320	CB	GLU	A	57	68.291	80.192	7.814	1.00	94.75
ATOM	321	CG	GLU	A	57	67.142	81.145	7.534	1.00	97.96
ATOM	322	CD	GLU	A	57	66.600	81.012	6.117	1.00	101.06
ATOM	323	OE1	GLU	A	57	66.106	79.919	5.760	1.00	102.91
ATOM	324	OE2	GLU	A	57	66.671	82.005	5.358	1.00	101.61
ATOM	325	C	GLU	A	57	67.686	78.728	9.764	1.00	91.34
ATOM	326	O	GLU	A	57	68.658	78.633	10.517	1.00	91.07
ATOM	327	N	ASN	A	58	66.428	78.787	10.200	1.00	88.53
ATOM	328	CA	ASN	A	58	66.119	78.725	11.620	1.00	86.10
ATOM	329	CB	ASN	A	58	64.713	79.256	11.899	1.00	84.84
ATOM	330	CG	ASN	A	58	64.712	80.734	12.255	1.00	84.41
ATOM	331	OD1	ASN	A	58	63.673	81.309	12.571	1.00	84.78
ATOM	332	ND2	ASN	A	58	65.883	81.353	12.209	1.00	84.89

107/396

Figure 2A-7

ATOM	333	C	ASN	A	58	66.261	77.297	12.131	1.00	85.39
ATOM	334	O	ASN	A	58	66.477	77.080	13.324	1.00	84.97
ATOM	335	N	VAL	A	59	66.143	76.325	11.229	1.00	84.39
ATOM	336	CA	VAL	A	59	66.308	74.926	11.612	1.00	84.80
ATOM	337	CB	VAL	A	59	65.666	73.948	10.587	1.00	84.81
ATOM	338	CG1	VAL	A	59	66.553	73.802	9.355	1.00	83.34
ATOM	339	CG2	VAL	A	59	65.445	72.592	11.235	1.00	84.78
ATOM	340	C	VAL	A	59	67.816	74.717	11.616	1.00	85.44
ATOM	341	O	VAL	A	59	68.353	73.958	12.418	1.00	86.18
ATOM	342	N	GLN	A	60	68.484	75.423	10.707	1.00	86.19
ATOM	343	CA	GLN	A	60	69.931	75.371	10.556	1.00	85.13
ATOM	344	CB	GLN	A	60	70.359	76.255	9.375	1.00	87.57
ATOM	345	CG	GLN	A	60	71.872	76.382	9.162	1.00	88.97
ATOM	346	CD	GLN	A	60	72.521	75.109	8.632	1.00	90.09
ATOM	347	OE1	GLN	A	60	73.737	75.064	8.415	1.00	90.19
ATOM	348	NE2	GLN	A	60	71.714	74.072	8.420	1.00	89.34
ATOM	349	C	GLN	A	60	70.594	75.857	11.839	1.00	83.50
ATOM	350	O	GLN	A	60	71.338	75.121	12.476	1.00	82.65
ATOM	351	N	ASN	A	61	70.321	77.101	12.211	1.00	82.96
ATOM	352	CA	ASN	A	61	70.894	77.675	13.419	1.00	82.67
ATOM	353	CB	ASN	A	61	70.297	79.059	13.679	1.00	84.20
ATOM	354	CG	ASN	A	61	70.894	80.131	12.782	1.00	86.24
ATOM	355	OD1	ASN	A	61	70.420	81.266	12.758	1.00	87.73
ATOM	356	ND2	ASN	A	61	71.947	79.779	12.049	1.00	85.87
ATOM	357	C	ASN	A	61	70.659	76.783	14.630	1.00	82.41
ATOM	358	O	ASN	A	61	71.555	76.598	15.458	1.00	80.93
ATOM	359	N	MET	A	62	69.453	76.229	14.725	1.00	81.52
ATOM	360	CA	MET	A	62	69.100	75.363	15.842	1.00	80.42
ATOM	361	CB	MET	A	62	67.606	75.020	15.810	1.00	79.01
ATOM	362	CG	MET	A	62	67.209	73.938	16.814	1.00	76.81
ATOM	363	SD	MET	A	62	65.472	73.445	16.763	1.00	71.30
ATOM	364	CE	MET	A	62	65.436	72.532	15.206	1.00	75.17
ATOM	365	C	MET	A	62	69.912	74.076	15.870	1.00	80.34
ATOM	366	O	MET	A	62	70.524	73.748	16.888	1.00	80.90
ATOM	367	N	ASN	A	63	69.923	73.344	14.760	1.00	80.00
ATOM	368	CA	ASN	A	63	70.662	72.088	14.715	1.00	80.18
ATOM	369	CB	ASN	A	63	70.457	71.382	13.366	1.00	82.56
ATOM	370	CG	ASN	A	63	70.972	72.193	12.189	1.00	87.14
ATOM	371	OD1	ASN	A	63	72.164	72.491	12.099	1.00	89.55
ATOM	372	ND2	ASN	A	63	70.072	72.553	11.275	1.00	88.42
ATOM	373	C	ASN	A	63	72.149	72.290	14.993	1.00	79.09
ATOM	374	O	ASN	A	63	72.798	71.422	15.570	1.00	78.18
ATOM	375	N	ASN	A	64	72.687	73.437	14.593	1.00	77.48
ATOM	376	CA	ASN	A	64	74.097	73.727	14.828	1.00	76.54
ATOM	377	CB	ASN	A	64	74.579	74.843	13.892	1.00	79.55
ATOM	378	CG	ASN	A	64	74.553	74.429	12.427	1.00	82.11
ATOM	379	OD1	ASN	A	64	75.074	73.375	12.062	1.00	82.94
ATOM	380	ND2	ASN	A	64	73.951	75.263	11.581	1.00	81.87
ATOM	381	C	ASN	A	64	74.336	74.132	16.287	1.00	74.58
ATOM	382	O	ASN	A	64	75.330	73.739	16.895	1.00	73.89
ATOM	383	N	ALA	A	65	73.426	74.926	16.840	1.00	72.42
ATOM	384	CA	ALA	A	65	73.546	75.359	18.227	1.00	70.26
ATOM	385	CB	ALA	A	65	72.474	76.393	18.556	1.00	68.51
ATOM	386	C	ALA	A	65	73.375	74.127	19.104	1.00	68.93
ATOM	387	O	ALA	A	65	73.974	74.021	20.177	1.00	67.92
ATOM	388	N	GLY	A	66	72.564	73.192	18.622	1.00	66.17

108/396

Figure 2A-8

ATOM	389	CA	GLY	A	66	72.320	71.970	19.358	1.00	66.18
ATOM	390	C	GLY	A	66	73.497	71.014	19.347	1.00	65.56
ATOM	391	O	GLY	A	66	73.778	70.371	20.352	1.00	67.52
ATOM	392	N	ASP	A	67	74.186	70.920	18.215	1.00	66.25
ATOM	393	CA	ASP	A	67	75.340	70.033	18.075	1.00	67.79
ATOM	394	CB	ASP	A	67	75.678	69.855	16.592	1.00	70.41
ATOM	395	CG	ASP	A	67	74.702	68.923	15.879	1.00	73.83
ATOM	396	OD1	ASP	A	67	73.471	69.061	16.087	1.00	71.64
ATOM	397	OD2	ASP	A	67	75.172	68.053	15.108	1.00	76.19
ATOM	398	C	ASP	A	67	76.561	70.554	18.829	1.00	67.60
ATOM	399	O	ASP	A	67	77.471	69.793	19.157	1.00	67.81
ATOM	400	N	LYS	A	68	76.576	71.859	19.084	1.00	67.23
ATOM	401	CA	LYS	A	68	77.656	72.502	19.823	1.00	67.11
ATOM	402	CB	LYS	A	68	77.602	74.023	19.608	1.00	68.36
ATOM	403	CG	LYS	A	68	78.747	74.803	20.235	1.00	68.98
ATOM	404	CD	LYS	A	68	79.236	75.922	19.314	1.00	71.67
ATOM	405	CE	LYS	A	68	79.856	75.356	18.022	1.00	73.96
ATOM	406	NZ	LYS	A	68	80.557	76.374	17.167	1.00	74.02
ATOM	407	C	LYS	A	68	77.468	72.159	21.308	1.00	66.21
ATOM	408	O	LYS	A	68	78.439	71.978	22.044	1.00	66.82
ATOM	409	N	TRP	A	69	76.210	72.060	21.730	1.00	63.72
ATOM	410	CA	TRP	A	69	75.878	71.718	23.106	1.00	63.60
ATOM	411	CB	TRP	A	69	74.389	71.978	23.361	1.00	64.44
ATOM	412	CG	TRP	A	69	73.844	71.371	24.635	1.00	63.91
ATOM	413	CD2	TRP	A	69	74.132	71.779	25.981	1.00	61.14
ATOM	414	CE2	TRP	A	69	73.408	70.919	26.841	1.00	62.62
ATOM	415	CE3	TRP	A	69	74.933	72.784	26.544	1.00	59.72
ATOM	416	CD1	TRP	A	69	72.981	70.312	24.732	1.00	62.16
ATOM	417	NE1	TRP	A	69	72.715	70.037	26.051	1.00	62.75
ATOM	418	CZ2	TRP	A	69	73.458	71.036	28.238	1.00	58.61
ATOM	419	CZ3	TRP	A	69	74.983	72.901	27.934	1.00	58.23
ATOM	420	CH2	TRP	A	69	74.248	72.029	28.764	1.00	60.27
ATOM	421	C	TRP	A	69	76.226	70.259	23.397	1.00	63.40
ATOM	422	O	TRP	A	69	76.802	69.947	24.439	1.00	61.39
ATOM	423	N	SER	A	70	75.887	69.370	22.467	1.00	63.14
ATOM	424	CA	SER	A	70	76.170	67.941	22.625	1.00	61.91
ATOM	425	CB	SER	A	70	75.532	67.145	21.491	1.00	61.57
ATOM	426	OG	SER	A	70	74.129	67.328	21.497	1.00	64.22
ATOM	427	C	SER	A	70	77.660	67.660	22.654	1.00	59.01
ATOM	428	O	SER	A	70	78.119	66.796	23.395	1.00	61.08
ATOM	429	N	ALA	A	71	78.406	68.389	21.837	1.00	57.98
ATOM	430	CA	ALA	A	71	79.850	68.236	21.771	1.00	58.78
ATOM	431	CB	ALA	A	71	80.391	69.007	20.578	1.00	58.94
ATOM	432	C	ALA	A	71	80.499	68.737	23.071	1.00	60.03
ATOM	433	O	ALA	A	71	81.512	68.208	23.517	1.00	59.29
ATOM	434	N	PHE	A	72	79.914	69.775	23.660	1.00	59.88
ATOM	435	CA	PHE	A	72	80.413	70.332	24.914	1.00	59.99
ATOM	436	CB	PHE	A	72	79.685	71.653	25.213	1.00	57.59
ATOM	437	CG	PHE	A	72	79.906	72.178	26.604	1.00	58.56
ATOM	438	CD1	PHE	A	72	81.167	72.601	27.017	1.00	58.71
ATOM	439	CD2	PHE	A	72	78.841	72.269	27.500	1.00	59.34
ATOM	440	CE1	PHE	A	72	81.369	73.112	28.300	1.00	59.03
ATOM	441	CE2	PHE	A	72	79.025	72.779	28.790	1.00	60.64
ATOM	442	CZ	PHE	A	72	80.296	73.202	29.190	1.00	60.01
ATOM	443	C	PHE	A	72	80.152	69.310	26.025	1.00	60.40
ATOM	444	O	PHE	A	72	81.037	68.997	26.826	1.00	60.24

109/396

Figure 2A-9

ATOM	445	N	LEU	A	73	78.934	68.773	26.035	1.00	60.11
ATOM	446	CA	LEU	A	73	78.508	67.798	27.032	1.00	61.07
ATOM	447	CB	LEU	A	73	77.036	67.446	26.808	1.00	60.54
ATOM	448	CG	LEU	A	73	76.095	67.442	28.011	1.00	58.89
ATOM	449	CD1	LEU	A	73	76.191	68.759	28.758	1.00	61.73
ATOM	450	CD2	LEU	A	73	74.674	67.222	27.523	1.00	57.29
ATOM	451	C	LEU	A	73	79.338	66.524	27.015	1.00	60.00
ATOM	452	O	LEU	A	73	79.514	65.877	28.047	1.00	61.58
ATOM	453	N	LYS	A	74	79.847	66.170	25.842	1.00	60.55
ATOM	454	CA	LYS	A	74	80.644	64.962	25.688	1.00	60.73
ATOM	455	CB	LYS	A	74	80.638	64.518	24.221	1.00	63.62
ATOM	456	CG	LYS	A	74	81.227	63.138	23.984	1.00	64.80
ATOM	457	CD	LYS	A	74	81.252	62.797	22.503	1.00	70.00
ATOM	458	CE	LYS	A	74	81.627	61.339	22.281	1.00	72.00
ATOM	459	NZ	LYS	A	74	82.912	60.993	22.957	1.00	75.14
ATOM	460	C	LYS	A	74	82.076	65.179	26.159	1.00	60.97
ATOM	461	O	LYS	A	74	82.667	64.312	26.802	1.00	59.43
ATOM	462	N	GLU	A	75	82.643	66.333	25.832	1.00	60.12
ATOM	463	CA	GLU	A	75	83.999	66.613	26.257	1.00	63.28
ATOM	464	CB	GLU	A	75	84.529	67.888	25.591	1.00	66.51
ATOM	465	CG	GLU	A	75	85.961	68.206	25.997	1.00	75.32
ATOM	466	CD	GLU	A	75	86.445	69.556	25.502	1.00	80.58
ATOM	467	OE1	GLU	A	75	87.628	69.888	25.754	1.00	83.10
ATOM	468	OE2	GLU	A	75	85.647	70.284	24.870	1.00	84.90
ATOM	469	C	GLU	A	75	84.000	66.783	27.778	1.00	64.02
ATOM	470	O	GLU	A	75	84.918	66.327	28.466	1.00	64.36
ATOM	471	N	GLN	A	76	82.960	67.434	28.293	1.00	60.36
ATOM	472	CA	GLN	A	76	82.839	67.676	29.721	1.00	59.54
ATOM	473	CB	GLN	A	76	81.713	68.671	29.979	1.00	55.33
ATOM	474	CG	GLN	A	76	82.013	70.066	29.458	1.00	52.65
ATOM	475	CD	GLN	A	76	83.169	70.714	30.197	1.00	53.62
ATOM	476	OE1	GLN	A	76	83.217	70.695	31.427	1.00	48.86
ATOM	477	NE2	GLN	A	76	84.104	71.295	29.451	1.00	50.80
ATOM	478	C	GLN	A	76	82.596	66.392	30.502	1.00	61.69
ATOM	479	O	GLN	A	76	83.021	66.260	31.651	1.00	62.42
ATOM	480	N	SER	A	77	81.903	65.449	29.879	1.00	62.55
ATOM	481	CA	SER	A	77	81.631	64.173	30.516	1.00	64.74
ATOM	482	CB	SER	A	77	80.596	63.393	29.711	1.00	66.34
ATOM	483	OG	SER	A	77	80.375	62.121	30.286	1.00	70.86
ATOM	484	C	SER	A	77	82.923	63.366	30.594	1.00	65.95
ATOM	485	O	SER	A	77	83.293	62.863	31.648	1.00	64.19
ATOM	486	N	THR	A	78	83.610	63.255	29.466	1.00	69.57
ATOM	487	CA	THR	A	78	84.851	62.503	29.403	1.00	74.17
ATOM	488	CB	THR	A	78	85.127	62.041	27.962	1.00	76.59
ATOM	489	OG1	THR	A	78	85.373	63.181	27.128	1.00	79.55
ATOM	490	CG2	THR	A	78	83.919	61.277	27.420	1.00	77.74
ATOM	491	C	THR	A	78	86.031	63.323	29.915	1.00	75.58
ATOM	492	O	THR	A	78	87.179	63.108	29.510	1.00	77.37
ATOM	493	N	LEU	A	79	85.736	64.259	30.810	1.00	74.94
ATOM	494	CA	LEU	A	79	86.746	65.123	31.404	1.00	73.63
ATOM	495	CB	LEU	A	79	86.636	66.534	30.831	1.00	72.34
ATOM	496	CG	LEU	A	79	87.830	67.481	30.969	1.00	70.71
ATOM	497	CD1	LEU	A	79	89.017	66.946	30.184	1.00	67.16
ATOM	498	CD2	LEU	A	79	87.440	68.853	30.454	1.00	70.99
ATOM	499	C	LEU	A	79	86.450	65.151	32.894	1.00	75.13
ATOM	500	O	LEU	A	79	87.281	65.555	33.702	1.00	74.18

110/396

Figure 2A-10

ATOM	501	N	ALA	A	80	85.244	64.716	33.243	1.00	76.89
ATOM	502	CA	ALA	A	80	84.806	64.665	34.628	1.00	78.89
ATOM	503	CB	ALA	A	80	83.302	64.865	34.706	1.00	78.74
ATOM	504	C	ALA	A	80	85.187	63.321	35.234	1.00	80.25
ATOM	505	O	ALA	A	80	85.214	63.170	36.455	1.00	79.67
ATOM	506	N	GLN	A	81	85.475	62.347	34.375	1.00	82.26
ATOM	507	CA	GLN	A	81	85.861	61.014	34.832	1.00	85.46
ATOM	508	CB	GLN	A	81	86.308	60.152	33.651	1.00	84.52
ATOM	509	CG	GLN	A	81	85.302	60.012	32.513	1.00	83.92
ATOM	510	CD	GLN	A	81	84.019	59.331	32.935	1.00	83.07
ATOM	511	OE1	GLN	A	81	84.013	58.500	33.844	1.00	82.48
ATOM	512	NE2	GLN	A	81	82.922	59.668	32.263	1.00	82.57
ATOM	513	C	GLN	A	81	87.026	61.155	35.809	1.00	88.10
ATOM	514	O	GLN	A	81	87.061	60.519	36.863	1.00	88.72
ATOM	515	N	MET	A	82	87.972	62.006	35.432	1.00	90.80
ATOM	516	CA	MET	A	82	89.169	62.287	36.215	1.00	93.67
ATOM	517	CB	MET	A	82	89.748	63.640	35.779	1.00	96.32
ATOM	518	CG	MET	A	82	91.094	63.998	36.397	1.00	100.94
ATOM	519	SD	MET	A	82	91.662	65.665	35.928	1.00	105.24
ATOM	520	CE	MET	A	82	91.659	66.498	37.533	1.00	103.93
ATOM	521	C	MET	A	82	88.967	62.295	37.731	1.00	93.99
ATOM	522	O	MET	A	82	89.854	61.871	38.472	1.00	94.66
ATOM	523	N	TYR	A	83	87.807	62.762	38.189	1.00	94.27
ATOM	524	CA	TYR	A	83	87.535	62.854	39.625	1.00	95.62
ATOM	525	CB	TYR	A	83	86.708	64.112	39.913	1.00	93.30
ATOM	526	CG	TYR	A	83	87.293	65.334	39.250	1.00	93.10
ATOM	527	CD1	TYR	A	83	86.980	65.649	37.925	1.00	93.21
ATOM	528	CE1	TYR	A	83	87.594	66.714	37.271	1.00	90.92
ATOM	529	CD2	TYR	A	83	88.233	66.124	39.907	1.00	92.00
ATOM	530	CE2	TYR	A	83	88.854	67.189	39.262	1.00	91.63
ATOM	531	CZ	TYR	A	83	88.530	67.475	37.946	1.00	90.95
ATOM	532	OH	TYR	A	83	89.157	68.509	37.301	1.00	89.32
ATOM	533	C	TYR	A	83	86.865	61.636	40.249	1.00	97.22
ATOM	534	O	TYR	A	83	85.655	61.445	40.127	1.00	96.98
ATOM	535	N	PRO	A	84	87.656	60.807	40.954	1.00	98.57
ATOM	536	CD	PRO	A	84	89.068	61.074	41.284	1.00	99.73
ATOM	537	CA	PRO	A	84	87.192	59.588	41.623	1.00	99.29
ATOM	538	CB	PRO	A	84	88.343	59.256	42.569	1.00	99.49
ATOM	539	CG	PRO	A	84	89.538	59.734	41.813	1.00	99.82
ATOM	540	C	PRO	A	84	85.881	59.796	42.369	1.00	99.69
ATOM	541	O	PRO	A	84	85.813	60.567	43.327	1.00	99.64
ATOM	542	N	LEU	A	85	84.843	59.106	41.916	1.00	99.80
ATOM	543	CA	LEU	A	85	83.532	59.200	42.535	1.00	100.71
ATOM	544	CB	LEU	A	85	82.550	58.265	41.815	1.00	101.54
ATOM	545	CG	LEU	A	85	82.885	56.767	41.723	1.00	103.35
ATOM	546	CD1	LEU	A	85	81.783	56.051	40.947	1.00	102.29
ATOM	547	CD2	LEU	A	85	84.230	56.556	41.032	1.00	103.08
ATOM	548	C	LEU	A	85	83.594	58.860	44.027	1.00	100.79
ATOM	549	O	LEU	A	85	82.905	59.482	44.838	1.00	99.73
ATOM	550	N	GLN	A	86	84.429	57.887	44.388	1.00	100.79
ATOM	551	CA	GLN	A	86	84.557	57.479	45.785	1.00	101.20
ATOM	552	CB	GLN	A	86	85.249	56.112	45.888	1.00	102.47
ATOM	553	CG	GLN	A	86	85.258	55.540	47.306	1.00	106.22
ATOM	554	CD	GLN	A	86	85.840	54.133	47.390	1.00	108.88
ATOM	555	OE1	GLN	A	86	87.014	53.911	47.088	1.00	110.53
ATOM	556	NE2	GLN	A	86	85.015	53.175	47.808	1.00	109.96

111/396

Figure 2A-11

ATOM	557	C	GLN	A	86	85.316	58.509	46.624	1.00	100.03
ATOM	558	O	GLN	A	86	84.989	58.732	47.792	1.00	99.96
ATOM	559	N	GLU	A	87	86.327	59.135	46.031	1.00	98.50
ATOM	560	CA	GLU	A	87	87.109	60.143	46.739	1.00	97.58
ATOM	561	CB	GLU	A	87	88.340	60.538	45.918	1.00	99.29
ATOM	562	CG	GLU	A	87	89.670	59.921	46.356	1.00	101.67
ATOM	563	CD	GLU	A	87	89.711	58.409	46.225	1.00	103.68
ATOM	564	OE1	GLU	A	87	89.257	57.714	47.161	1.00	103.82
ATOM	565	OE2	GLU	A	87	90.193	57.915	45.180	1.00	103.75
ATOM	566	C	GLU	A	87	86.265	61.389	46.995	1.00	96.57
ATOM	567	O	GLU	A	87	86.775	62.396	47.481	1.00	96.59
ATOM	568	N	ILE	A	88	84.976	61.316	46.669	1.00	96.20
ATOM	569	CA	ILE	A	88	84.071	62.451	46.847	1.00	95.49
ATOM	570	CB	ILE	A	88	83.125	62.605	45.633	1.00	94.73
ATOM	571	CG2	ILE	A	88	82.265	63.853	45.800	1.00	92.94
ATOM	572	CG1	ILE	A	88	83.942	62.681	44.337	1.00	94.67
ATOM	573	CD1	ILE	A	88	84.910	63.859	44.262	1.00	92.86
ATOM	574	C	ILE	A	88	83.222	62.364	48.114	1.00	95.19
ATOM	575	O	ILE	A	88	82.637	61.324	48.415	1.00	95.50
ATOM	576	N	GLN	A	89	83.149	63.480	48.835	1.00	94.16
ATOM	577	CA	GLN	A	89	82.398	63.565	50.082	1.00	93.97
ATOM	578	CB	GLN	A	89	83.266	64.239	51.147	1.00	96.05
ATOM	579	CG	GLN	A	89	82.506	64.757	52.357	1.00	98.00
ATOM	580	CD	GLN	A	89	83.368	65.642	53.242	1.00	99.64
ATOM	581	OE1	GLN	A	89	84.364	65.190	53.810	1.00	98.69
ATOM	582	NE2	GLN	A	89	82.992	66.913	53.357	1.00	100.18
ATOM	583	C	GLN	A	89	81.085	64.325	49.942	1.00	92.85
ATOM	584	O	GLN	A	89	80.017	63.796	50.256	1.00	92.80
ATOM	585	N	ASN	A	90	81.176	65.574	49.493	1.00	91.82
ATOM	586	CA	ASN	A	90	80.007	66.434	49.305	1.00	90.00
ATOM	587	CB	ASN	A	90	80.455	67.773	48.718	1.00	88.93
ATOM	588	CG	ASN	A	90	79.384	68.837	48.808	1.00	90.31
ATOM	589	OD1	ASN	A	90	78.247	68.620	48.382	1.00	90.69
ATOM	590	ND2	ASN	A	90	79.758	69.989	49.362	1.00	89.32
ATOM	591	C	ASN	A	90	79.006	65.756	48.361	1.00	89.13
ATOM	592	O	ASN	A	90	79.260	65.633	47.164	1.00	89.62
ATOM	593	N	LEU	A	91	77.873	65.315	48.901	1.00	87.01
ATOM	594	CA	LEU	A	91	76.859	64.633	48.100	1.00	84.76
ATOM	595	CB	LEU	A	91	75.720	64.130	48.997	1.00	83.70
ATOM	596	CG	LEU	A	91	76.074	63.035	50.008	1.00	84.16
ATOM	597	CD1	LEU	A	91	77.070	63.572	51.022	1.00	85.49
ATOM	598	CD2	LEU	A	91	74.816	62.559	50.713	1.00	83.88
ATOM	599	C	LEU	A	91	76.291	65.509	46.984	1.00	83.87
ATOM	600	O	LEU	A	91	75.891	65.009	45.930	1.00	84.10
ATOM	601	N	THR	A	92	76.255	66.815	47.213	1.00	81.65
ATOM	602	CA	THR	A	92	75.742	67.729	46.208	1.00	80.13
ATOM	603	CB	THR	A	92	75.638	69.155	46.755	1.00	80.10
ATOM	604	OG1	THR	A	92	74.813	69.150	47.925	1.00	82.97
ATOM	605	CG2	THR	A	92	75.028	70.086	45.713	1.00	79.36
ATOM	606	C	THR	A	92	76.662	67.737	44.993	1.00	80.19
ATOM	607	O	THR	A	92	76.191	67.826	43.853	1.00	80.97
ATOM	608	N	VAL	A	93	77.971	67.646	45.230	1.00	76.90
ATOM	609	CA	VAL	A	93	78.915	67.644	44.126	1.00	74.33
ATOM	610	CB	VAL	A	93	80.339	68.059	44.561	1.00	74.63
ATOM	611	CG1	VAL	A	93	80.284	69.378	45.312	1.00	74.78
ATOM	612	CG2	VAL	A	93	80.970	66.978	45.394	1.00	76.02

112/396

Figure 2A-12

ATOM	613	C	VAL	A	93	78.973	66.265	43.503	1.00	72.24
ATOM	614	O	VAL	A	93	79.331	66.129	42.336	1.00	71.84
ATOM	615	N	LYS	A	94	78.615	65.240	44.273	1.00	70.34
ATOM	616	CA	LYS	A	94	78.623	63.881	43.740	1.00	70.81
ATOM	617	CB	LYS	A	94	78.433	62.830	44.850	1.00	70.96
ATOM	618	CG	LYS	A	94	78.844	61.419	44.402	1.00	73.05
ATOM	619	CD	LYS	A	94	78.465	60.311	45.391	1.00	76.49
ATOM	620	CE	LYS	A	94	76.986	59.920	45.268	1.00	78.53
ATOM	621	NZ	LYS	A	94	76.611	58.721	46.089	1.00	75.61
ATOM	622	C	LYS	A	94	77.483	63.767	42.726	1.00	68.94
ATOM	623	O	LYS	A	94	77.649	63.182	41.660	1.00	68.54
ATOM	624	N	LEU	A	95	76.327	64.334	43.069	1.00	67.45
ATOM	625	CA	LEU	A	95	75.166	64.316	42.180	1.00	66.32
ATOM	626	CB	LEU	A	95	74.021	65.151	42.762	1.00	63.75
ATOM	627	CG	LEU	A	95	73.287	64.566	43.963	1.00	62.63
ATOM	628	CD1	LEU	A	95	72.254	65.573	44.469	1.00	61.49
ATOM	629	CD2	LEU	A	95	72.633	63.248	43.565	1.00	58.53
ATOM	630	C	LEU	A	95	75.543	64.881	40.821	1.00	64.55
ATOM	631	O	LEU	A	95	75.398	64.209	39.801	1.00	66.30
ATOM	632	N	GLN	A	96	76.022	66.122	40.819	1.00	63.21
ATOM	633	CA	GLN	A	96	76.424	66.800	39.590	1.00	60.69
ATOM	634	CB	GLN	A	96	76.995	68.169	39.920	1.00	58.58
ATOM	635	CG	GLN	A	96	75.958	69.204	40.200	1.00	58.51
ATOM	636	CD	GLN	A	96	76.539	70.399	40.910	1.00	58.33
ATOM	637	OE1	GLN	A	96	76.760	70.360	42.116	1.00	59.96
ATOM	638	NE2	GLN	A	96	76.801	71.464	40.167	1.00	56.20
ATOM	639	C	GLN	A	96	77.464	65.996	38.833	1.00	60.85
ATOM	640	O	GLN	A	96	77.341	65.766	37.629	1.00	58.49
ATOM	641	N	LEU	A	97	78.493	65.576	39.556	1.00	61.80
ATOM	642	CA	LEU	A	97	79.573	64.801	38.977	1.00	62.94
ATOM	643	CB	LEU	A	97	80.612	64.514	40.054	1.00	64.08
ATOM	644	CG	LEU	A	97	82.008	64.048	39.653	1.00	66.97
ATOM	645	CD1	LEU	A	97	82.676	65.088	38.750	1.00	68.41
ATOM	646	CD2	LEU	A	97	82.824	63.834	40.923	1.00	66.32
ATOM	647	C	LEU	A	97	78.995	63.506	38.428	1.00	64.54
ATOM	648	O	LEU	A	97	79.357	63.055	37.344	1.00	63.86
ATOM	649	N	GLN	A	98	78.073	62.922	39.181	1.00	67.80
ATOM	650	CA	GLN	A	98	77.433	61.676	38.787	1.00	70.42
ATOM	651	CB	GLN	A	98	76.423	61.254	39.861	1.00	71.77
ATOM	652	CG	GLN	A	98	75.981	59.800	39.788	1.00	77.72
ATOM	653	CD	GLN	A	98	75.189	59.373	41.018	1.00	80.79
ATOM	654	OE1	GLN	A	98	74.090	59.875	41.276	1.00	82.19
ATOM	655	NE2	GLN	A	98	75.750	58.446	41.786	1.00	81.55
ATOM	656	C	GLN	A	98	76.736	61.843	37.435	1.00	70.21
ATOM	657	O	GLN	A	98	76.974	61.076	36.499	1.00	69.62
ATOM	658	N	ALA	A	99	75.881	62.852	37.332	1.00	68.84
ATOM	659	CA	ALA	A	99	75.165	63.101	36.092	1.00	70.01
ATOM	660	CB	ALA	A	99	74.353	64.377	36.215	1.00	66.95
ATOM	661	C	ALA	A	99	76.129	63.199	34.907	1.00	72.32
ATOM	662	O	ALA	A	99	75.911	62.577	33.863	1.00	72.81
ATOM	663	N	LEU	A	100	77.202	63.965	35.086	1.00	72.80
ATOM	664	CA	LEU	A	100	78.197	64.180	34.043	1.00	73.52
ATOM	665	CB	LEU	A	100	79.147	65.310	34.460	1.00	70.38
ATOM	666	CG	LEU	A	100	78.694	66.738	34.147	1.00	67.25
ATOM	667	CD1	LEU	A	100	79.759	67.742	34.565	1.00	64.22
ATOM	668	CD2	LEU	A	100	78.436	66.851	32.657	1.00	64.69

113/396

Figure 2A-13

ATOM	669	C	LEU	A	100	79.032	62.995	33.547	1.00	76.54
ATOM	670	O	LEU	A	100	79.164	62.801	32.335	1.00	76.36
ATOM	671	N	GLN	A	101	79.604	62.206	34.455	1.00	79.19
ATOM	672	CA	GLN	A	101	80.446	61.093	34.021	1.00	81.30
ATOM	673	CB	GLN	A	101	81.545	60.813	35.051	1.00	80.60
ATOM	674	CG	GLN	A	101	81.082	60.642	36.471	1.00	82.38
ATOM	675	CD	GLN	A	101	82.244	60.368	37.403	1.00	83.28
ATOM	676	OE1	GLN	A	101	82.914	59.337	37.289	1.00	84.47
ATOM	677	NE2	GLN	A	101	82.502	61.295	38.322	1.00	81.04
ATOM	678	C	GLN	A	101	79.721	59.805	33.671	1.00	83.04
ATOM	679	O	GLN	A	101	80.217	58.705	33.920	1.00	84.24
ATOM	680	N	GLN	A	102	78.552	59.959	33.064	1.00	84.21
ATOM	681	CA	GLN	A	102	77.734	58.835	32.639	1.00	85.45
ATOM	682	CB	GLN	A	102	76.265	59.177	32.872	1.00	86.92
ATOM	683	CG	GLN	A	102	75.289	58.057	32.633	1.00	91.09
ATOM	684	CD	GLN	A	102	73.854	58.520	32.820	1.00	94.74
ATOM	685	OE1	GLN	A	102	73.481	59.006	33.893	1.00	96.04
ATOM	686	NE2	GLN	A	102	73.041	58.378	31.775	1.00	94.23
ATOM	687	C	GLN	A	102	78.020	58.656	31.147	1.00	85.36
ATOM	688	O	GLN	A	102	77.588	59.472	30.331	1.00	85.23
ATOM	689	N	ASN	A	103	78.754	57.600	30.794	1.00	84.82
ATOM	690	CA	ASN	A	103	79.115	57.357	29.397	1.00	85.12
ATOM	691	CB	ASN	A	103	80.177	56.258	29.294	1.00	85.12
ATOM	692	CG	ASN	A	103	81.506	56.668	29.900	1.00	85.17
ATOM	693	OD1	ASN	A	103	81.914	57.827	29.804	1.00	83.24
ATOM	694	ND2	ASN	A	103	82.192	55.704	30.506	1.00	86.52
ATOM	695	C	ASN	A	103	77.955	57.008	28.473	1.00	85.31
ATOM	696	O	ASN	A	103	77.796	57.616	27.415	1.00	86.45
ATOM	697	N	GLY	A	104	77.155	56.020	28.859	1.00	84.66
ATOM	698	CA	GLY	A	104	76.029	55.630	28.031	1.00	82.09
ATOM	699	C	GLY	A	104	76.447	54.849	26.799	1.00	81.02
ATOM	700	O	GLY	A	104	77.160	53.855	26.904	1.00	80.56
ATOM	701	N	SER	A	105	76.004	55.305	25.630	1.00	80.48
ATOM	702	CA	SER	A	105	76.316	54.641	24.369	1.00	80.61
ATOM	703	CB	SER	A	105	75.393	55.159	23.264	1.00	81.43
ATOM	704	OG	SER	A	105	74.037	54.897	23.586	1.00	86.85
ATOM	705	C	SER	A	105	77.767	54.813	23.943	1.00	79.44
ATOM	706	O	SER	A	105	78.318	53.952	23.246	1.00	77.44
ATOM	707	N	SER	A	106	78.379	55.923	24.357	1.00	78.32
ATOM	708	CA	SER	A	106	79.776	56.204	24.020	1.00	76.74
ATOM	709	CB	SER	A	106	80.210	57.561	24.590	1.00	77.89
ATOM	710	OG	SER	A	106	80.410	57.495	25.997	1.00	78.59
ATOM	711	C	SER	A	106	80.682	55.109	24.577	1.00	74.81
ATOM	712	O	SER	A	106	81.875	55.072	24.285	1.00	75.47
ATOM	713	N	VAL	A	107	80.104	54.219	25.380	1.00	73.50
ATOM	714	CA	VAL	A	107	80.846	53.118	25.978	1.00	71.66
ATOM	715	CB	VAL	A	107	80.179	52.639	27.287	1.00	71.02
ATOM	716	CG1	VAL	A	107	79.058	51.657	26.978	1.00	70.32
ATOM	717	CG2	VAL	A	107	81.208	52.016	28.195	1.00	68.94
ATOM	718	C	VAL	A	107	80.907	51.957	24.992	1.00	71.74
ATOM	719	O	VAL	A	107	81.498	50.921	25.276	1.00	71.88
ATOM	720	N	LEU	A	108	80.285	52.141	23.833	1.00	72.10
ATOM	721	CA	LEU	A	108	80.269	51.120	22.789	1.00	73.27
ATOM	722	CB	LEU	A	108	78.895	51.066	22.104	1.00	73.83
ATOM	723	CG	LEU	A	108	77.702	50.466	22.856	1.00	73.31
ATOM	724	CD1	LEU	A	108	76.418	50.777	22.093	1.00	72.78

114/396

Figure 2A-14

ATOM	725	CD2	LEU	A	108	77.892	48.960	23.018	1.00	71.31
ATOM	726	C	LEU	A	108	81.326	51.414	21.733	1.00	73.60
ATOM	727	O	LEU	A	108	81.745	52.558	21.564	1.00	72.45
ATOM	728	N	SER	A	109	81.749	50.372	21.021	1.00	73.87
ATOM	729	CA	SER	A	109	82.735	50.528	19.964	1.00	75.39
ATOM	730	CB	SER	A	109	83.090	49.173	19.369	1.00	72.84
ATOM	731	OG	SER	A	109	82.024	48.693	18.578	1.00	73.28
ATOM	732	C	SER	A	109	82.085	51.401	18.895	1.00	77.33
ATOM	733	O	SER	A	109	80.864	51.514	18.846	1.00	79.54
ATOM	734	N	GLU	A	110	82.894	52.007	18.035	1.00	78.57
ATOM	735	CA	GLU	A	110	82.374	52.880	16.989	1.00	78.82
ATOM	736	CB	GLU	A	110	83.529	53.432	16.151	1.00	81.77
ATOM	737	CG	GLU	A	110	83.111	54.428	15.076	1.00	88.52
ATOM	738	CD	GLU	A	110	82.226	55.549	15.613	1.00	91.76
ATOM	739	OE1	GLU	A	110	81.031	55.292	15.893	1.00	93.60
ATOM	740	OE2	GLU	A	110	82.728	56.686	15.762	1.00	93.54
ATOM	741	C	GLU	A	110	81.349	52.200	16.080	1.00	77.16
ATOM	742	O	GLU	A	110	80.313	52.785	15.765	1.00	75.62
ATOM	743	N	ASP	A	111	81.635	50.970	15.664	1.00	74.97
ATOM	744	CA	ASP	A	111	80.728	50.234	14.789	1.00	73.35
ATOM	745	CB	ASP	A	111	81.418	48.990	14.217	1.00	75.23
ATOM	746	CG	ASP	A	111	82.569	49.336	13.276	1.00	77.85
ATOM	747	OD1	ASP	A	111	82.454	50.335	12.526	1.00	77.70
ATOM	748	OD2	ASP	A	111	83.582	48.600	13.275	1.00	78.25
ATOM	749	C	ASP	A	111	79.430	49.820	15.482	1.00	72.26
ATOM	750	O	ASP	A	111	78.412	49.620	14.821	1.00	71.34
ATOM	751	N	LYS	A	112	79.470	49.682	16.806	1.00	69.42
ATOM	752	CA	LYS	A	112	78.284	49.303	17.566	1.00	66.50
ATOM	753	CB	LYS	A	112	78.676	48.790	18.960	1.00	66.44
ATOM	754	CG	LYS	A	112	79.401	47.430	18.984	1.00	67.17
ATOM	755	CD	LYS	A	112	78.506	46.289	18.528	1.00	65.55
ATOM	756	CE	LYS	A	112	79.191	44.931	18.682	1.00	67.23
ATOM	757	NZ	LYS	A	112	79.504	44.587	20.098	1.00	61.17
ATOM	758	C	LYS	A	112	77.359	50.517	17.705	1.00	63.84
ATOM	759	O	LYS	A	112	76.163	50.437	17.435	1.00	58.93
ATOM	760	N	SER	A	113	77.936	51.637	18.128	1.00	61.54
ATOM	761	CA	SER	A	113	77.199	52.877	18.309	1.00	60.23
ATOM	762	CB	SER	A	113	78.147	53.984	18.770	1.00	58.54
ATOM	763	OG	SER	A	113	78.646	53.706	20.061	1.00	63.58
ATOM	764	C	SER	A	113	76.528	53.302	17.014	1.00	58.67
ATOM	765	O	SER	A	113	75.400	53.792	17.018	1.00	59.20
ATOM	766	N	LYS	A	114	77.238	53.117	15.911	1.00	57.74
ATOM	767	CA	LYS	A	114	76.731	53.480	14.603	1.00	59.50
ATOM	768	CB	LYS	A	114	77.831	53.276	13.546	1.00	62.52
ATOM	769	CG	LYS	A	114	77.716	54.160	12.290	1.00	66.59
ATOM	770	CD	LYS	A	114	76.471	53.831	11.468	1.00	71.77
ATOM	771	CE	LYS	A	114	76.321	54.756	10.266	1.00	73.32
ATOM	772	NZ	LYS	A	114	76.084	56.163	10.679	1.00	73.57
ATOM	773	C	LYS	A	114	75.515	52.610	14.288	1.00	57.76
ATOM	774	O	LYS	A	114	74.468	53.111	13.870	1.00	56.73
ATOM	775	N	ARG	A	115	75.651	51.306	14.502	1.00	56.62
ATOM	776	CA	ARG	A	115	74.554	50.385	14.216	1.00	56.98
ATOM	777	CB	ARG	A	115	75.018	48.934	14.387	1.00	57.56
ATOM	778	CG	ARG	A	115	73.950	47.889	14.135	1.00	57.02
ATOM	779	CD	ARG	A	115	73.382	47.981	12.726	1.00	61.86
ATOM	780	NE	ARG	A	115	72.331	46.987	12.512	1.00	63.02

115/396

Figure 2A-15

ATOM	781	CZ	ARG	A	115	71.484	46.991	11.489	1.00	62.78
ATOM	782	NH1	ARG	A	115	70.565	46.040	11.392	1.00	63.16
ATOM	783	NH2	ARG	A	115	71.546	47.944	10.567	1.00	63.93
ATOM	784	C	ARG	A	115	73.356	50.679	15.112	1.00	55.89
ATOM	785	O	ARG	A	115	72.222	50.734	14.633	1.00	54.32
ATOM	786	N	LEU	A	116	73.606	50.893	16.402	1.00	55.29
ATOM	787	CA	LEU	A	116	72.523	51.191	17.332	1.00	55.31
ATOM	788	CB	LEU	A	116	73.046	51.395	18.761	1.00	52.95
ATOM	789	CG	LEU	A	116	72.005	51.924	19.765	1.00	54.56
ATOM	790	CD1	LEU	A	116	70.831	50.957	19.825	1.00	55.14
ATOM	791	CD2	LEU	A	116	72.618	52.095	21.158	1.00	49.17
ATOM	792	C	LEU	A	116	71.783	52.445	16.881	1.00	55.89
ATOM	793	O	LEU	A	116	70.553	52.468	16.876	1.00	59.67
ATOM	794	N	ASN	A	117	72.519	53.484	16.494	1.00	54.04
ATOM	795	CA	ASN	A	117	71.873	54.714	16.053	1.00	53.18
ATOM	796	CB	ASN	A	117	72.910	55.829	15.840	1.00	55.18
ATOM	797	CG	ASN	A	117	73.383	56.437	17.155	1.00	60.23
ATOM	798	OD1	ASN	A	117	72.674	56.375	18.173	1.00	61.54
ATOM	799	ND2	ASN	A	117	74.573	57.039	17.143	1.00	58.53
ATOM	800	C	ASN	A	117	71.056	54.483	14.786	1.00	50.03
ATOM	801	O	ASN	A	117	69.972	55.041	14.626	1.00	48.24
ATOM	802	N	THR	A	118	71.579	53.653	13.894	1.00	49.26
ATOM	803	CA	THR	A	118	70.883	53.315	12.668	1.00	51.07
ATOM	804	CB	THR	A	118	71.764	52.409	11.789	1.00	53.79
ATOM	805	OG1	THR	A	118	72.946	53.127	11.424	1.00	57.45
ATOM	806	CG2	THR	A	118	71.040	51.996	10.531	1.00	54.26
ATOM	807	C	THR	A	118	69.579	52.606	13.051	1.00	50.56
ATOM	808	O	THR	A	118	68.505	52.990	12.606	1.00	52.60
ATOM	809	N	ILE	A	119	69.664	51.597	13.907	1.00	49.00
ATOM	810	CA	ILE	A	119	68.460	50.897	14.330	1.00	47.66
ATOM	811	CB	ILE	A	119	68.770	49.753	15.315	1.00	44.90
ATOM	812	CG2	ILE	A	119	67.479	49.183	15.875	1.00	43.67
ATOM	813	CG1	ILE	A	119	69.519	48.638	14.586	1.00	43.89
ATOM	814	CD1	ILE	A	119	69.930	47.502	15.493	1.00	49.56
ATOM	815	C	ILE	A	119	67.447	51.827	14.979	1.00	47.18
ATOM	816	O	ILE	A	119	66.255	51.719	14.727	1.00	49.10
ATOM	817	N	LEU	A	120	67.898	52.737	15.829	1.00	48.44
ATOM	818	CA	LEU	A	120	66.944	53.649	16.456	1.00	50.68
ATOM	819	CB	LEU	A	120	67.640	54.533	17.503	1.00	48.38
ATOM	820	CG	LEU	A	120	68.113	53.821	18.783	1.00	52.60
ATOM	821	CD1	LEU	A	120	69.029	54.741	19.616	1.00	49.34
ATOM	822	CD2	LEU	A	120	66.893	53.394	19.604	1.00	49.45
ATOM	823	C	LEU	A	120	66.265	54.517	15.384	1.00	51.10
ATOM	824	O	LEU	A	120	65.035	54.637	15.356	1.00	49.70
ATOM	825	N	ASN	A	121	67.057	55.099	14.486	1.00	51.11
ATOM	826	CA	ASN	A	121	66.486	55.953	13.450	1.00	51.82
ATOM	827	CB	ASN	A	121	67.594	56.624	12.634	1.00	52.02
ATOM	828	CG	ASN	A	121	68.345	57.672	13.444	1.00	59.03
ATOM	829	OD1	ASN	A	121	67.735	58.466	14.168	1.00	58.92
ATOM	830	ND2	ASN	A	121	69.670	57.682	13.327	1.00	60.28
ATOM	831	C	ASN	A	121	65.537	55.198	12.544	1.00	50.14
ATOM	832	O	ASN	A	121	64.499	55.729	12.141	1.00	50.64
ATOM	833	N	THR	A	122	65.883	53.954	12.243	1.00	48.51
ATOM	834	CA	THR	A	122	65.054	53.124	11.389	1.00	46.86
ATOM	835	CB	THR	A	122	65.778	51.814	11.020	1.00	45.74
ATOM	836	OG1	THR	A	122	67.079	52.128	10.514	1.00	44.00

116/396

Figure 2A-16

ATOM	837	CG2	THR	A	122	64.998	51.043	9.943	1.00	41.71
ATOM	838	C	THR	A	122	63.724	52.798	12.067	1.00	49.58
ATOM	839	O	THR	A	122	62.675	53.002	11.466	1.00	51.60
ATOM	840	N	MET	A	123	63.756	52.308	13.311	1.00	47.65
ATOM	841	CA	MET	A	123	62.513	51.971	14.003	1.00	45.98
ATOM	842	CB	MET	A	123	62.766	51.450	15.435	1.00	45.68
ATOM	843	CG	MET	A	123	63.473	50.097	15.553	1.00	44.72
ATOM	844	SD	MET	A	123	63.322	49.349	17.218	1.00	46.36
ATOM	845	CE	MET	A	123	64.398	50.469	18.217	1.00	42.83
ATOM	846	C	MET	A	123	61.657	53.219	14.095	1.00	45.95
ATOM	847	O	MET	A	123	60.435	53.181	13.936	1.00	45.26
ATOM	848	N	SER	A	124	62.308	54.338	14.363	1.00	45.05
ATOM	849	CA	SER	A	124	61.580	55.579	14.500	1.00	45.46
ATOM	850	CB	SER	A	124	62.522	56.690	14.939	1.00	43.29
ATOM	851	OG	SER	A	124	61.779	57.854	15.208	1.00	47.27
ATOM	852	C	SER	A	124	60.859	56.007	13.224	1.00	43.55
ATOM	853	O	SER	A	124	59.721	56.480	13.270	1.00	42.34
ATOM	854	N	THR	A	125	61.521	55.847	12.090	1.00	44.66
ATOM	855	CA	THR	A	125	60.920	56.269	10.843	1.00	49.23
ATOM	856	CB	THR	A	125	61.975	56.456	9.725	1.00	49.01
ATOM	857	OG1	THR	A	125	62.571	55.197	9.416	1.00	59.59
ATOM	858	CG2	THR	A	125	63.057	57.418	10.172	1.00	47.07
ATOM	859	C	THR	A	125	59.827	55.331	10.368	1.00	49.32
ATOM	860	O	THR	A	125	58.792	55.809	9.924	1.00	50.12
ATOM	861	N	ILE	A	126	60.016	54.012	10.473	1.00	48.00
ATOM	862	CA	ILE	A	126	58.949	53.130	10.013	1.00	47.22
ATOM	863	CB	ILE	A	126	59.329	51.620	10.062	1.00	51.68
ATOM	864	CG2	ILE	A	126	60.781	51.409	9.693	1.00	51.02
ATOM	865	CG1	ILE	A	126	59.042	51.052	11.433	1.00	50.67
ATOM	866	CD1	ILE	A	126	57.704	50.365	11.494	1.00	57.08
ATOM	867	C	ILE	A	126	57.707	53.368	10.867	1.00	46.60
ATOM	868	O	ILE	A	126	56.591	53.175	10.391	1.00	46.53
ATOM	869	N	TYR	A	127	57.893	53.801	12.118	1.00	41.34
ATOM	870	CA	TYR	A	127	56.761	54.086	13.007	1.00	39.34
ATOM	871	CB	TYR	A	127	57.240	54.306	14.459	1.00	37.78
ATOM	872	CG	TYR	A	127	56.113	54.598	15.440	1.00	34.70
ATOM	873	CD1	TYR	A	127	55.676	55.904	15.701	1.00	36.21
ATOM	874	CE1	TYR	A	127	54.603	56.137	16.554	1.00	31.09
ATOM	875	CD2	TYR	A	127	55.443	53.551	16.064	1.00	35.75
ATOM	876	CE2	TYR	A	127	54.378	53.775	16.902	1.00	30.86
ATOM	877	CZ	TYR	A	127	53.963	55.044	17.146	1.00	32.70
ATOM	878	OH	TYR	A	127	52.901	55.180	18.009	1.00	35.06
ATOM	879	C	TYR	A	127	55.990	55.337	12.584	1.00	40.68
ATOM	880	O	TYR	A	127	54.756	55.379	12.621	1.00	42.01
ATOM	881	N	SER	A	128	56.717	56.375	12.198	1.00	40.32
ATOM	882	CA	SER	A	128	56.047	57.616	11.838	1.00	44.51
ATOM	883	CB	SER	A	128	56.917	58.818	12.196	1.00	42.95
ATOM	884	OG	SER	A	128	58.089	58.814	11.410	1.00	51.68
ATOM	885	C	SER	A	128	55.706	57.691	10.370	1.00	42.67
ATOM	886	O	SER	A	128	54.981	58.572	9.967	1.00	43.94
ATOM	887	N	THR	A	129	56.191	56.741	9.586	1.00	43.66
ATOM	888	CA	THR	A	129	55.951	56.782	8.162	1.00	47.52
ATOM	889	CB	THR	A	129	57.283	57.089	7.443	1.00	48.58
ATOM	890	OG1	THR	A	129	57.005	57.666	6.168	1.00	61.81
ATOM	891	CG2	THR	A	129	58.119	55.837	7.272	1.00	41.94
ATOM	892	C	THR	A	129	55.291	55.525	7.597	1.00	47.49

117/396

Figure 2A-17

ATOM	893	O	THR	A	129	54.911	55.479	6.429	1.00	49.22
ATOM	894	N	GLY	A	130	55.137	54.512	8.438	1.00	46.83
ATOM	895	CA	GLY	A	130	54.511	53.286	7.994	1.00	45.36
ATOM	896	C	GLY	A	130	53.039	53.513	7.736	1.00	47.05
ATOM	897	O	GLY	A	130	52.408	54.381	8.350	1.00	44.82
ATOM	898	N	LYS	A	131	52.478	52.741	6.818	1.00	47.58
ATOM	899	CA	LYS	A	131	51.066	52.887	6.511	1.00	50.27
ATOM	900	CB	LYS	A	131	50.868	53.930	5.400	1.00	50.99
ATOM	901	CG	LYS	A	131	51.673	53.685	4.146	1.00	59.48
ATOM	902	CD	LYS	A	131	51.453	54.825	3.147	1.00	64.82
ATOM	903	CE	LYS	A	131	51.719	56.192	3.790	1.00	67.13
ATOM	904	NZ	LYS	A	131	51.384	57.347	2.903	1.00	68.87
ATOM	905	C	LYS	A	131	50.409	51.579	6.117	1.00	49.00
ATOM	906	O	LYS	A	131	51.071	50.623	5.726	1.00	49.46
ATOM	907	N	VAL	A	132	49.095	51.525	6.239	1.00	49.08
ATOM	908	CA	VAL	A	132	48.392	50.315	5.854	1.00	52.73
ATOM	909	CB	VAL	A	132	47.622	49.685	7.049	1.00	51.23
ATOM	910	CG1	VAL	A	132	48.592	49.293	8.130	1.00	50.88
ATOM	911	CG2	VAL	A	132	46.609	50.648	7.592	1.00	49.52
ATOM	912	C	VAL	A	132	47.424	50.739	4.767	1.00	53.85
ATOM	913	O	VAL	A	132	47.019	51.901	4.713	1.00	54.37
ATOM	914	N	CYS	A	133	47.055	49.818	3.891	1.00	54.83
ATOM	915	CA	CYS	A	133	46.136	50.188	2.827	1.00	56.77
ATOM	916	C	CYS	A	133	44.875	49.336	2.852	1.00	55.53
ATOM	917	O	CYS	A	133	44.895	48.189	3.298	1.00	56.58
ATOM	918	CB	CYS	A	133	46.820	50.069	1.464	1.00	56.58
ATOM	919	SG	CYS	A	133	48.427	50.922	1.285	1.00	65.06
ATOM	920	N	ASN	A	134	43.779	49.923	2.383	1.00	54.76
ATOM	921	CA	ASN	A	134	42.495	49.254	2.319	1.00	57.69
ATOM	922	CB	ASN	A	134	41.456	50.206	1.745	1.00	58.07
ATOM	923	CG	ASN	A	134	40.078	49.586	1.681	1.00	60.24
ATOM	924	OD1	ASN	A	134	39.938	48.388	1.460	1.00	57.02
ATOM	925	ND2	ASN	A	134	39.049	50.407	1.859	1.00	63.28
ATOM	926	C	ASN	A	134	42.579	48.003	1.438	1.00	59.84
ATOM	927	O	ASN	A	134	43.078	48.055	0.312	1.00	60.55
ATOM	928	N	PRO	A	135	42.084	46.859	1.940	1.00	60.76
ATOM	929	CD	PRO	A	135	41.464	46.618	3.254	1.00	61.99
ATOM	930	CA	PRO	A	135	42.133	45.624	1.155	1.00	63.06
ATOM	931	CB	PRO	A	135	41.523	44.587	2.098	1.00	64.33
ATOM	932	CG	PRO	A	135	41.772	45.163	3.474	1.00	65.00
ATOM	933	C	PRO	A	135	41.349	45.740	-0.156	1.00	64.46
ATOM	934	O	PRO	A	135	41.722	45.142	-1.162	1.00	64.26
ATOM	935	N	ASP	A	136	40.269	46.516	-0.140	1.00	65.50
ATOM	936	CA	ASP	A	136	39.448	46.688	-1.328	1.00	66.22
ATOM	937	CB	ASP	A	136	37.973	46.898	-0.940	1.00	69.38
ATOM	938	CG	ASP	A	136	37.564	48.367	-0.919	1.00	77.68
ATOM	939	OD1	ASP	A	136	37.620	48.991	0.167	1.00	80.49
ATOM	940	OD2	ASP	A	136	37.186	48.897	-1.995	1.00	81.68
ATOM	941	C	ASP	A	136	39.935	47.837	-2.212	1.00	64.97
ATOM	942	O	ASP	A	136	39.386	48.075	-3.293	1.00	66.57
ATOM	943	N	ASN	A	137	40.967	48.545	-1.757	1.00	60.64
ATOM	944	CA	ASN	A	137	41.528	49.651	-2.528	1.00	54.85
ATOM	945	CB	ASN	A	137	40.674	50.907	-2.360	1.00	52.69
ATOM	946	CG	ASN	A	137	41.180	52.069	-3.190	1.00	51.54
ATOM	947	OD1	ASN	A	137	40.592	53.150	-3.183	1.00	53.79
ATOM	948	ND2	ASN	A	137	42.274	51.856	-3.909	1.00	50.98

118/396

Figure 2A-18

ATOM	949	C	ASN	A	137	42.961	49.930	-2.093	1.00	52.24
ATOM	950	O	ASN	A	137	43.203	50.747	-1.211	1.00	49.03
ATOM	951	N	PRO	A	138	43.931	49.250	-2.730	1.00	50.93
ATOM	952	CD	PRO	A	138	43.664	48.237	-3.767	1.00	49.28
ATOM	953	CA	PRO	A	138	45.370	49.354	-2.477	1.00	50.16
ATOM	954	CB	PRO	A	138	45.968	48.444	-3.542	1.00	49.69
ATOM	955	CG	PRO	A	138	44.912	47.393	-3.719	1.00	47.48
ATOM	956	C	PRO	A	138	45.934	50.767	-2.563	1.00	51.38
ATOM	957	O	PRO	A	138	47.076	51.004	-2.177	1.00	51.91
ATOM	958	N	GLN	A	139	45.139	51.701	-3.073	1.00	50.05
ATOM	959	CA	GLN	A	139	45.597	53.077	-3.212	1.00	49.94
ATOM	960	CB	GLN	A	139	45.143	53.648	-4.565	1.00	49.98
ATOM	961	CG	GLN	A	139	45.975	53.159	-5.759	1.00	48.90
ATOM	962	CD	GLN	A	139	45.796	51.680	-6.046	1.00	48.92
ATOM	963	OE1	GLN	A	139	46.769	50.923	-6.105	1.00	51.65
ATOM	964	NE2	GLN	A	139	44.547	51.257	-6.223	1.00	48.33
ATOM	965	C	GLN	A	139	45.126	53.969	-2.052	1.00	50.68
ATOM	966	O	GLN	A	139	45.564	55.109	-1.908	1.00	46.80
ATOM	967	N	GLU	A	140	44.232	53.442	-1.227	1.00	50.21
ATOM	968	CA	GLU	A	140	43.765	54.194	-0.080	1.00	55.32
ATOM	969	CB	GLU	A	140	42.296	53.890	0.209	1.00	57.65
ATOM	970	CG	GLU	A	140	41.651	54.910	1.125	1.00	64.24
ATOM	971	CD	GLU	A	140	40.426	54.371	1.829	1.00	69.34
ATOM	972	OE1	GLU	A	140	39.520	53.852	1.142	1.00	71.41
ATOM	973	OE2	GLU	A	140	40.370	54.474	3.074	1.00	74.64
ATOM	974	C	GLU	A	140	44.639	53.692	1.060	1.00	55.83
ATOM	975	O	GLU	A	140	44.465	52.577	1.543	1.00	57.65
ATOM	976	N	CYS	A	141	45.605	54.500	1.465	1.00	56.74
ATOM	977	CA	CYS	A	141	46.507	54.098	2.528	1.00	59.52
ATOM	978	C	CYS	A	141	46.506	55.135	3.650	1.00	59.02
ATOM	979	O	CYS	A	141	46.466	56.340	3.402	1.00	61.88
ATOM	980	CB	CYS	A	141	47.915	53.911	1.959	1.00	60.12
ATOM	981	SG	CYS	A	141	48.021	52.773	0.527	1.00	63.46
ATOM	982	N	LEU	A	142	46.537	54.655	4.885	1.00	56.42
ATOM	983	CA	LEU	A	142	46.510	55.522	6.054	1.00	54.06
ATOM	984	CB	LEU	A	142	45.300	55.184	6.927	1.00	56.85
ATOM	985	CG	LEU	A	142	43.892	55.206	6.322	1.00	59.41
ATOM	986	CD1	LEU	A	142	42.944	54.469	7.257	1.00	57.01
ATOM	987	CD2	LEU	A	142	43.425	56.649	6.099	1.00	56.77
ATOM	988	C	LEU	A	142	47.759	55.396	6.919	1.00	52.34
ATOM	989	O	LEU	A	142	48.337	54.316	7.047	1.00	51.96
ATOM	990	N	LEU	A	143	48.164	56.514	7.505	1.00	49.20
ATOM	991	CA	LEU	A	143	49.295	56.547	8.412	1.00	47.92
ATOM	992	CB	LEU	A	143	49.992	57.918	8.397	1.00	47.85
ATOM	993	CG	LEU	A	143	50.886	58.332	7.221	1.00	51.86
ATOM	994	CD1	LEU	A	143	50.148	58.130	5.911	1.00	57.42
ATOM	995	CD2	LEU	A	143	51.277	59.796	7.368	1.00	52.90
ATOM	996	C	LEU	A	143	48.643	56.359	9.770	1.00	46.19
ATOM	997	O	LEU	A	143	47.420	56.454	9.893	1.00	41.29
ATOM	998	N	LEU	A	144	49.454	56.094	10.789	1.00	46.33
ATOM	999	CA	LEU	A	144	48.926	55.942	12.140	1.00	45.18
ATOM	1000	CB	LEU	A	144	50.064	55.683	13.134	1.00	43.33
ATOM	1001	CG	LEU	A	144	49.572	55.694	14.574	1.00	45.90
ATOM	1002	CD1	LEU	A	144	48.501	54.606	14.718	1.00	44.19
ATOM	1003	CD2	LEU	A	144	50.733	55.464	15.545	1.00	45.65
ATOM	1004	C	LEU	A	144	48.243	57.255	12.512	1.00	41.13

119/396

Figure 2A-19

ATOM	1005	O	LEU	A	144	47.129	57.274	13.033	1.00	43.69
ATOM	1006	N	GLU	A	145	48.937	58.351	12.243	1.00	40.73
ATOM	1007	CA	GLU	A	145	48.435	59.683	12.563	1.00	45.47
ATOM	1008	CB	GLU	A	145	49.353	60.347	13.591	1.00	44.17
ATOM	1009	CG	GLU	A	145	49.001	61.795	13.913	1.00	46.95
ATOM	1010	CD	GLU	A	145	47.625	61.967	14.549	1.00	50.23
ATOM	1011	OE1	GLU	A	145	47.100	61.019	15.169	1.00	51.42
ATOM	1012	OE2	GLU	A	145	47.068	63.081	14.448	1.00	58.80
ATOM	1013	C	GLU	A	145	48.341	60.594	11.342	1.00	46.80
ATOM	1014	O	GLU	A	145	49.357	60.938	10.739	1.00	47.22
ATOM	1015	N	PRO	A	146	47.120	60.980	10.952	1.00	49.40
ATOM	1016	CD	PRO	A	146	46.878	61.999	9.906	1.00	51.83
ATOM	1017	CA	PRO	A	146	45.866	60.598	11.600	1.00	51.79
ATOM	1018	CB	PRO	A	146	45.005	61.834	11.396	1.00	51.49
ATOM	1019	CG	PRO	A	146	45.363	62.209	9.965	1.00	48.47
ATOM	1020	C	PRO	A	146	45.387	59.421	10.768	1.00	53.37
ATOM	1021	O	PRO	A	146	46.162	58.856	10.002	1.00	59.06
ATOM	1022	N	GLY	A	147	44.135	59.031	10.889	1.00	52.09
ATOM	1023	CA	GLY	A	147	43.698	57.936	10.041	1.00	49.44
ATOM	1024	C	GLY	A	147	43.423	56.705	10.850	1.00	48.35
ATOM	1025	O	GLY	A	147	42.278	56.412	11.179	1.00	48.36
ATOM	1026	N	LEU	A	148	44.484	55.980	11.175	1.00	45.67
ATOM	1027	CA	LEU	A	148	44.345	54.789	11.979	1.00	43.56
ATOM	1028	CB	LEU	A	148	45.678	54.043	12.006	1.00	42.22
ATOM	1029	CG	LEU	A	148	45.720	52.716	11.237	1.00	45.41
ATOM	1030	CD1	LEU	A	148	44.832	52.738	10.011	1.00	42.58
ATOM	1031	CD2	LEU	A	148	47.157	52.416	10.862	1.00	47.86
ATOM	1032	C	LEU	A	148	43.911	55.245	13.374	1.00	43.14
ATOM	1033	O	LEU	A	148	43.033	54.637	13.996	1.00	45.01
ATOM	1034	N	ASN	A	149	44.508	56.329	13.855	1.00	41.83
ATOM	1035	CA	ASN	A	149	44.154	56.868	15.162	1.00	42.69
ATOM	1036	CB	ASN	A	149	45.059	58.052	15.527	1.00	43.48
ATOM	1037	CG	ASN	A	149	46.415	57.626	16.093	1.00	45.50
ATOM	1038	OD1	ASN	A	149	47.338	58.432	16.139	1.00	42.75
ATOM	1039	ND2	ASN	A	149	46.533	56.369	16.535	1.00	39.67
ATOM	1040	C	ASN	A	149	42.720	57.367	15.124	1.00	45.08
ATOM	1041	O	ASN	A	149	41.951	57.162	16.076	1.00	44.60
ATOM	1042	N	GLU	A	150	42.354	58.030	14.026	1.00	45.41
ATOM	1043	CA	GLU	A	150	41.002	58.579	13.910	1.00	46.09
ATOM	1044	CB	GLU	A	150	40.840	59.367	12.610	1.00	49.42
ATOM	1045	CG	GLU	A	150	39.524	60.144	12.526	1.00	57.23
ATOM	1046	CD	GLU	A	150	38.324	59.257	12.182	1.00	62.26
ATOM	1047	OE1	GLU	A	150	37.177	59.634	12.525	1.00	63.79
ATOM	1048	OE2	GLU	A	150	38.529	58.192	11.552	1.00	62.45
ATOM	1049	C	GLU	A	150	39.984	57.463	13.983	1.00	45.82
ATOM	1050	O	GLU	A	150	38.935	57.602	14.620	1.00	45.64
ATOM	1051	N	ILE	A	151	40.306	56.348	13.336	1.00	46.15
ATOM	1052	CA	ILE	A	151	39.437	55.180	13.338	1.00	45.70
ATOM	1053	CB	ILE	A	151	39.974	54.068	12.409	1.00	47.91
ATOM	1054	CG2	ILE	A	151	39.220	52.772	12.670	1.00	45.66
ATOM	1055	CG1	ILE	A	151	39.856	54.482	10.942	1.00	46.22
ATOM	1056	CD1	ILE	A	151	40.489	53.472	10.006	1.00	42.79
ATOM	1057	C	ILE	A	151	39.351	54.564	14.726	1.00	45.96
ATOM	1058	O	ILE	A	151	38.264	54.355	15.252	1.00	46.23
ATOM	1059	N	MET	A	152	40.508	54.249	15.307	1.00	46.22
ATOM	1060	CA	MET	A	152	40.542	53.605	16.613	1.00	43.96

120/396

Figure 2A-20

ATOM	1061	CB	MET	A	152	41.988	53.263	16.999	1.00	46.29
ATOM	1062	CG	MET	A	152	42.665	52.281	16.033	1.00	44.44
ATOM	1063	SD	MET	A	152	41.625	50.802	15.743	1.00	45.46
ATOM	1064	CE	MET	A	152	41.803	49.959	17.393	1.00	34.48
ATOM	1065	C	MET	A	152	39.870	54.408	17.710	1.00	43.70
ATOM	1066	O	MET	A	152	39.435	53.852	18.728	1.00	41.89
ATOM	1067	N	ALA	A	153	39.747	55.711	17.495	1.00	42.79
ATOM	1068	CA	ALA	A	153	39.119	56.560	18.492	1.00	43.58
ATOM	1069	CB	ALA	A	153	39.858	57.890	18.579	1.00	41.92
ATOM	1070	C	ALA	A	153	37.639	56.819	18.235	1.00	47.66
ATOM	1071	O	ALA	A	153	36.870	57.036	19.186	1.00	46.65
ATOM	1072	N	ASN	A	154	37.221	56.770	16.971	1.00	46.91
ATOM	1073	CA	ASN	A	154	35.828	57.093	16.663	1.00	50.34
ATOM	1074	CB	ASN	A	154	35.792	58.336	15.766	1.00	50.34
ATOM	1075	CG	ASN	A	154	36.543	59.519	16.374	1.00	53.80
ATOM	1076	OD1	ASN	A	154	37.592	59.931	15.877	1.00	57.26
ATOM	1077	ND2	ASN	A	154	36.013	60.058	17.461	1.00	55.06
ATOM	1078	C	ASN	A	154	34.918	56.020	16.063	1.00	51.27
ATOM	1079	O	ASN	A	154	33.696	56.128	16.170	1.00	51.82
ATOM	1080	N	SER	A	155	35.495	54.987	15.460	1.00	50.44
ATOM	1081	CA	SER	A	155	34.706	53.939	14.829	1.00	50.66
ATOM	1082	CB	SER	A	155	35.595	53.097	13.912	1.00	49.98
ATOM	1083	OG	SER	A	155	34.914	51.931	13.478	1.00	47.52
ATOM	1084	C	SER	A	155	33.973	53.021	15.791	1.00	52.39
ATOM	1085	O	SER	A	155	34.474	52.723	16.876	1.00	53.19
ATOM	1086	N	LEU	A	156	32.784	52.568	15.377	1.00	53.08
ATOM	1087	CA	LEU	A	156	31.975	51.656	16.185	1.00	51.35
ATOM	1088	CB	LEU	A	156	30.618	52.274	16.542	1.00	51.20
ATOM	1089	CG	LEU	A	156	30.583	53.265	17.712	1.00	51.63
ATOM	1090	CD1	LEU	A	156	31.601	54.354	17.487	1.00	54.80
ATOM	1091	CD2	LEU	A	156	29.198	53.883	17.831	1.00	56.92
ATOM	1092	C	LEU	A	156	31.747	50.357	15.439	1.00	51.62
ATOM	1093	O	LEU	A	156	30.889	49.561	15.819	1.00	52.91
ATOM	1094	N	ASP	A	157	32.508	50.145	14.371	1.00	52.39
ATOM	1095	CA	ASP	A	157	32.380	48.923	13.588	1.00	52.43
ATOM	1096	CB	ASP	A	157	32.511	49.217	12.101	1.00	55.30
ATOM	1097	CG	ASP	A	157	32.532	47.950	11.273	1.00	60.74
ATOM	1098	OD1	ASP	A	157	31.456	47.496	10.841	1.00	66.67
ATOM	1099	OD2	ASP	A	157	33.623	47.383	11.079	1.00	64.61
ATOM	1100	C	ASP	A	157	33.458	47.913	13.984	1.00	51.68
ATOM	1101	O	ASP	A	157	34.642	48.141	13.777	1.00	53.84
ATOM	1102	N	TYR	A	158	33.038	46.791	14.539	1.00	49.69
ATOM	1103	CA	TYR	A	158	33.960	45.757	14.972	1.00	51.30
ATOM	1104	CB	TYR	A	158	33.168	44.509	15.376	1.00	47.99
ATOM	1105	CG	TYR	A	158	33.988	43.415	16.024	1.00	48.13
ATOM	1106	CD1	TYR	A	158	34.091	43.324	17.411	1.00	48.05
ATOM	1107	CE1	TYR	A	158	34.831	42.300	18.016	1.00	46.71
ATOM	1108	CD2	TYR	A	158	34.652	42.459	15.253	1.00	45.70
ATOM	1109	CE2	TYR	A	158	35.396	41.442	15.849	1.00	42.73
ATOM	1110	CZ	TYR	A	158	35.477	41.369	17.229	1.00	44.97
ATOM	1111	OH	TYR	A	158	36.205	40.364	17.828	1.00	48.58
ATOM	1112	C	TYR	A	158	34.999	45.391	13.910	1.00	53.20
ATOM	1113	O	TYR	A	158	36.198	45.341	14.198	1.00	53.30
ATOM	1114	N	ASN	A	159	34.551	45.143	12.682	1.00	52.58
ATOM	1115	CA	ASN	A	159	35.481	44.750	11.625	1.00	51.65
ATOM	1116	CB	ASN	A	159	34.716	44.220	10.414	1.00	52.14

121/396

Figure 2A-21

ATOM	1117	CG	ASN	A	159	33.812	43.063	10.772	1.00	55.50
ATOM	1118	OD1	ASN	A	159	34.215	42.142	11.492	1.00	54.18
ATOM	1119	ND2	ASN	A	159	32.580	43.096	10.265	1.00	54.02
ATOM	1120	C	ASN	A	159	36.462	45.815	11.172	1.00	47.34
ATOM	1121	O	ASN	A	159	37.616	45.513	10.897	1.00	46.53
ATOM	1122	N	GLU	A	160	36.008	47.058	11.081	1.00	46.21
ATOM	1123	CA	GLU	A	160	36.890	48.139	10.663	1.00	46.62
ATOM	1124	CB	GLU	A	160	36.079	49.422	10.469	1.00	45.86
ATOM	1125	CG	GLU	A	160	36.883	50.552	9.869	1.00	50.10
ATOM	1126	CD	GLU	A	160	36.158	51.876	9.944	1.00	54.51
ATOM	1127	OE1	GLU	A	160	36.603	52.840	9.280	1.00	56.85
ATOM	1128	OE2	GLU	A	160	35.142	51.957	10.670	1.00	58.04
ATOM	1129	C	GLU	A	160	37.988	48.349	11.733	1.00	44.77
ATOM	1130	O	GLU	A	160	39.171	48.485	11.410	1.00	44.02
ATOM	1131	N	ARG	A	161	37.589	48.376	13.002	1.00	44.83
ATOM	1132	CA	ARG	A	161	38.546	48.545	14.092	1.00	46.69
ATOM	1133	CB	ARG	A	161	37.831	48.597	15.452	1.00	43.36
ATOM	1134	CG	ARG	A	161	36.942	49.804	15.665	1.00	46.24
ATOM	1135	CD	ARG	A	161	36.368	49.811	17.081	1.00	45.54
ATOM	1136	NE	ARG	A	161	37.437	50.038	18.041	1.00	43.25
ATOM	1137	CZ	ARG	A	161	37.839	51.239	18.429	1.00	41.31
ATOM	1138	NH1	ARG	A	161	37.244	52.330	17.960	1.00	38.33
ATOM	1139	NH2	ARG	A	161	38.883	51.351	19.230	1.00	40.36
ATOM	1140	C	ARG	A	161	39.535	47.379	14.081	1.00	45.90
ATOM	1141	O	ARG	A	161	40.727	47.561	14.321	1.00	45.53
ATOM	1142	N	LEU	A	162	39.036	46.181	13.793	1.00	45.31
ATOM	1143	CA	LEU	A	162	39.891	45.006	13.766	1.00	46.80
ATOM	1144	CB	LEU	A	162	39.057	43.724	13.625	1.00	48.46
ATOM	1145	CG	LEU	A	162	39.870	42.443	13.400	1.00	52.64
ATOM	1146	CD1	LEU	A	162	40.800	42.247	14.583	1.00	52.10
ATOM	1147	CD2	LEU	A	162	38.951	41.227	13.240	1.00	52.05
ATOM	1148	C	LEU	A	162	40.859	45.120	12.606	1.00	47.94
ATOM	1149	O	LEU	A	162	42.051	44.816	12.736	1.00	49.60
ATOM	1150	N	TRP	A	163	40.352	45.546	11.455	1.00	46.70
ATOM	1151	CA	TRP	A	163	41.215	45.696	10.300	1.00	44.72
ATOM	1152	CB	TRP	A	163	40.444	46.265	9.107	1.00	44.32
ATOM	1153	CG	TRP	A	163	41.409	46.737	8.063	1.00	43.32
ATOM	1154	CD2	TRP	A	163	41.779	48.093	7.794	1.00	42.14
ATOM	1155	CE2	TRP	A	163	42.824	48.062	6.848	1.00	43.69
ATOM	1156	CE3	TRP	A	163	41.330	49.333	8.266	1.00	44.77
ATOM	1157	CD1	TRP	A	163	42.219	45.956	7.284	1.00	43.94
ATOM	1158	NE1	TRP	A	163	43.076	46.745	6.555	1.00	45.91
ATOM	1159	CZ2	TRP	A	163	43.434	49.231	6.358	1.00	46.63
ATOM	1160	CZ3	TRP	A	163	41.935	50.498	7.778	1.00	49.11
ATOM	1161	CH2	TRP	A	163	42.975	50.434	6.833	1.00	45.91
ATOM	1162	C	TRP	A	163	42.390	46.625	10.610	1.00	42.50
ATOM	1163	O	TRP	A	163	43.534	46.319	10.297	1.00	43.42
ATOM	1164	N	ALA	A	164	42.092	47.776	11.203	1.00	42.86
ATOM	1165	CA	ALA	A	164	43.124	48.755	11.543	1.00	40.52
ATOM	1166	CB	ALA	A	164	42.451	50.075	11.985	1.00	34.25
ATOM	1167	C	ALA	A	164	44.110	48.250	12.625	1.00	40.01
ATOM	1168	O	ALA	A	164	45.325	48.424	12.502	1.00	42.03
ATOM	1169	N	TRP	A	165	43.588	47.630	13.677	1.00	41.38
ATOM	1170	CA	TRP	A	165	44.422	47.098	14.772	1.00	42.00
ATOM	1171	CB	TRP	A	165	43.532	46.438	15.837	1.00	39.13
ATOM	1172	CG	TRP	A	165	44.226	46.012	17.106	1.00	40.79

122/396

Figure 2A-22

ATOM	1173	CD2	TRP	A	165	44.844	44.739	17.367	1.00	40.50
ATOM	1174	CE2	TRP	A	165	45.348	44.781	18.693	1.00	41.14
ATOM	1175	CE3	TRP	A	165	45.021	43.572	16.612	1.00	41.00
ATOM	1176	CD1	TRP	A	165	44.377	46.752	18.254	1.00	42.61
ATOM	1177	NE1	TRP	A	165	45.049	46.014	19.210	1.00	43.44
ATOM	1178	CZ2	TRP	A	165	46.019	43.701	19.274	1.00	42.24
ATOM	1179	CZ3	TRP	A	165	45.693	42.492	17.192	1.00	43.60
ATOM	1180	CH2	TRP	A	165	46.185	42.568	18.512	1.00	42.02
ATOM	1181	C	TRP	A	165	45.445	46.080	14.262	1.00	40.90
ATOM	1182	O	TRP	A	165	46.640	46.253	14.469	1.00	42.37
ATOM	1183	N	GLU	A	166	44.963	45.032	13.591	1.00	42.70
ATOM	1184	CA	GLU	A	166	45.795	43.953	13.036	1.00	41.42
ATOM	1185	CB	GLU	A	166	44.884	42.832	12.505	1.00	47.33
ATOM	1186	CG	GLU	A	166	45.586	41.728	11.704	1.00	46.79
ATOM	1187	CD	GLU	A	166	46.604	40.928	12.533	1.00	49.94
ATOM	1188	OE1	GLU	A	166	46.507	40.925	13.774	1.00	49.37
ATOM	1189	OE2	GLU	A	166	47.493	40.285	11.944	1.00	47.47
ATOM	1190	C	GLU	A	166	46.738	44.393	11.920	1.00	43.17
ATOM	1191	O	GLU	A	166	47.897	43.941	11.850	1.00	41.48
ATOM	1192	N	SER	A	167	46.244	45.257	11.035	1.00	40.45
ATOM	1193	CA	SER	A	167	47.062	45.745	9.924	1.00	43.46
ATOM	1194	CB	SER	A	167	46.210	46.593	8.965	1.00	45.87
ATOM	1195	OG	SER	A	167	45.210	45.800	8.353	1.00	51.72
ATOM	1196	C	SER	A	167	48.248	46.574	10.430	1.00	44.40
ATOM	1197	O	SER	A	167	49.353	46.491	9.887	1.00	45.57
ATOM	1198	N	TRP	A	168	48.015	47.386	11.458	1.00	42.01
ATOM	1199	CA	TRP	A	168	49.089	48.197	12.016	1.00	42.12
ATOM	1200	CB	TRP	A	168	48.579	49.055	13.185	1.00	41.93
ATOM	1201	CG	TRP	A	168	49.642	49.920	13.785	1.00	43.24
ATOM	1202	CD2	TRP	A	168	50.458	50.875	13.100	1.00	42.81
ATOM	1203	CE2	TRP	A	168	51.322	51.455	14.060	1.00	45.07
ATOM	1204	CE3	TRP	A	168	50.546	51.297	11.770	1.00	42.01
ATOM	1205	CD1	TRP	A	168	50.031	49.956	15.098	1.00	43.66
ATOM	1206	NE1	TRP	A	168	51.041	50.876	15.270	1.00	42.50
ATOM	1207	CZ2	TRP	A	168	52.260	52.442	13.730	1.00	42.94
ATOM	1208	CZ3	TRP	A	168	51.480	52.281	11.435	1.00	41.74
ATOM	1209	CH2	TRP	A	168	52.324	52.840	12.416	1.00	45.74
ATOM	1210	C	TRP	A	168	50.163	47.249	12.517	1.00	38.64
ATOM	1211	O	TRP	A	168	51.322	47.397	12.183	1.00	39.76
ATOM	1212	N	ARG	A	169	49.766	46.249	13.298	1.00	40.00
ATOM	1213	CA	ARG	A	169	50.738	45.302	13.835	1.00	40.67
ATOM	1214	CB	ARG	A	169	50.101	44.523	14.991	1.00	40.48
ATOM	1215	CG	ARG	A	169	49.783	45.427	16.175	1.00	39.02
ATOM	1216	CD	ARG	A	169	48.841	44.797	17.161	1.00	38.95
ATOM	1217	NE	ARG	A	169	48.733	45.630	18.357	1.00	42.15
ATOM	1218	CZ	ARG	A	169	48.093	46.795	18.401	1.00	40.36
ATOM	1219	NH1	ARG	A	169	48.057	47.497	19.529	1.00	36.29
ATOM	1220	NH2	ARG	A	169	47.465	47.250	17.328	1.00	36.67
ATOM	1221	C	ARG	A	169	51.307	44.355	12.793	1.00	41.05
ATOM	1222	O	ARG	A	169	52.448	43.930	12.881	1.00	40.91
ATOM	1223	N	SER	A	170	50.513	44.031	11.787	1.00	47.66
ATOM	1224	CA	SER	A	170	50.987	43.120	10.767	1.00	50.26
ATOM	1225	CB	SER	A	170	49.808	42.490	10.036	1.00	52.69
ATOM	1226	OG	SER	A	170	50.255	41.307	9.408	1.00	62.66
ATOM	1227	C	SER	A	170	51.933	43.765	9.767	1.00	50.16
ATOM	1228	O	SER	A	170	52.935	43.165	9.395	1.00	50.18

123/396

Figure 2A-23

ATOM	1229	N	GLU	A	171	51.635	44.987	9.336	1.00	52.37
ATOM	1230	CA	GLU	A	171	52.504	45.656	8.372	1.00	53.96
ATOM	1231	CB	GLU	A	171	51.711	46.646	7.519	1.00	61.95
ATOM	1232	CG	GLU	A	171	51.279	46.085	6.184	1.00	70.95
ATOM	1233	CD	GLU	A	171	50.291	44.961	6.336	1.00	76.26
ATOM	1234	OE1	GLU	A	171	49.114	45.255	6.636	1.00	80.75
ATOM	1235	OE2	GLU	A	171	50.693	43.787	6.171	1.00	79.07
ATOM	1236	C	GLU	A	171	53.715	46.376	8.955	1.00	52.82
ATOM	1237	O	GLU	A	171	54.818	46.245	8.431	1.00	54.65
ATOM	1238	N	VAL	A	172	53.545	47.149	10.018	1.00	48.92
ATOM	1239	CA	VAL	A	172	54.709	47.836	10.543	1.00	49.08
ATOM	1240	CB	VAL	A	172	54.379	49.313	10.932	1.00	51.59
ATOM	1241	CG1	VAL	A	172	53.598	49.976	9.818	1.00	52.69
ATOM	1242	CG2	VAL	A	172	53.591	49.365	12.214	1.00	57.56
ATOM	1243	C	VAL	A	172	55.320	47.105	11.721	1.00	46.06
ATOM	1244	O	VAL	A	172	56.533	46.965	11.805	1.00	49.16
ATOM	1245	N	GLY	A	173	54.492	46.620	12.631	1.00	46.62
ATOM	1246	CA	GLY	A	173	55.031	45.920	13.786	1.00	45.33
ATOM	1247	C	GLY	A	173	56.038	44.864	13.393	1.00	45.17
ATOM	1248	O	GLY	A	173	57.115	44.756	13.981	1.00	47.09
ATOM	1249	N	LYS	A	174	55.698	44.076	12.381	1.00	45.70
ATOM	1250	CA	LYS	A	174	56.595	43.025	11.931	1.00	45.31
ATOM	1251	CB	LYS	A	174	55.914	42.150	10.880	1.00	47.06
ATOM	1252	CG	LYS	A	174	54.813	41.274	11.444	1.00	46.88
ATOM	1253	CD	LYS	A	174	54.345	40.323	10.380	1.00	48.74
ATOM	1254	CE	LYS	A	174	53.191	39.478	10.856	1.00	50.64
ATOM	1255	NZ	LYS	A	174	52.924	38.386	9.873	1.00	56.98
ATOM	1256	C	LYS	A	174	57.903	43.560	11.382	1.00	44.05
ATOM	1257	O	LYS	A	174	58.914	42.877	11.427	1.00	44.50
ATOM	1258	N	GLN	A	175	57.891	44.774	10.842	1.00	44.49
ATOM	1259	CA	GLN	A	175	59.123	45.347	10.320	1.00	43.22
ATOM	1260	CB	GLN	A	175	58.843	46.645	9.582	1.00	44.13
ATOM	1261	CG	GLN	A	175	57.988	46.502	8.340	1.00	45.21
ATOM	1262	CD	GLN	A	175	57.941	47.793	7.571	1.00	45.83
ATOM	1263	OE1	GLN	A	175	58.986	48.345	7.213	1.00	50.54
ATOM	1264	NE2	GLN	A	175	56.742	48.298	7.320	1.00	45.95
ATOM	1265	C	GLN	A	175	60.019	45.653	11.509	1.00	42.33
ATOM	1266	O	GLN	A	175	61.235	45.641	11.411	1.00	42.15
ATOM	1267	N	LEU	A	176	59.385	45.930	12.636	1.00	44.10
ATOM	1268	CA	LEU	A	176	60.086	46.271	13.847	1.00	45.75
ATOM	1269	CB	LEU	A	176	59.133	47.005	14.775	1.00	45.31
ATOM	1270	CG	LEU	A	176	59.187	48.530	14.869	1.00	50.74
ATOM	1271	CD1	LEU	A	176	59.936	49.141	13.713	1.00	47.61
ATOM	1272	CD2	LEU	A	176	57.765	49.047	14.946	1.00	47.25
ATOM	1273	C	LEU	A	176	60.675	45.078	14.578	1.00	47.81
ATOM	1274	O	LEU	A	176	61.640	45.225	15.316	1.00	47.62
ATOM	1275	N	ARG	A	177	60.096	43.899	14.382	1.00	49.37
ATOM	1276	CA	ARG	A	177	60.568	42.720	15.094	1.00	50.25
ATOM	1277	CB	ARG	A	177	59.805	41.472	14.634	1.00	51.24
ATOM	1278	CG	ARG	A	177	60.208	40.198	15.367	1.00	53.40
ATOM	1279	CD	ARG	A	177	59.943	40.266	16.873	1.00	53.93
ATOM	1280	NE	ARG	A	177	60.651	39.198	17.583	1.00	51.95
ATOM	1281	CZ	ARG	A	177	60.065	38.286	18.358	1.00	51.91
ATOM	1282	NH1	ARG	A	177	60.800	37.356	18.961	1.00	50.97
ATOM	1283	NH2	ARG	A	177	58.751	38.303	18.538	1.00	42.74
ATOM	1284	C	ARG	A	177	62.072	42.500	14.991	1.00	50.86

124/396

Figure 2A-24

ATOM	1285	O	ARG	A	177	62.757	42.417	16.010	1.00	49.46
ATOM	1286	N	PRO	A	178	62.610	42.418	13.761	1.00	50.74
ATOM	1287	CD	PRO	A	178	61.915	42.573	12.477	1.00	47.66
ATOM	1288	CA	PRO	A	178	64.044	42.208	13.539	1.00	50.33
ATOM	1289	CB	PRO	A	178	64.173	42.297	12.022	1.00	48.41
ATOM	1290	CG	PRO	A	178	62.855	41.900	11.544	1.00	48.57
ATOM	1291	C	PRO	A	178	64.904	43.270	14.222	1.00	50.54
ATOM	1292	O	PRO	A	178	65.893	42.958	14.888	1.00	47.36
ATOM	1293	N	LEU	A	179	64.524	44.528	14.018	1.00	47.70
ATOM	1294	CA	LEU	A	179	65.250	45.651	14.582	1.00	48.04
ATOM	1295	CB	LEU	A	179	64.674	46.969	14.041	1.00	46.54
ATOM	1296	CG	LEU	A	179	64.691	47.050	12.508	1.00	47.80
ATOM	1297	CD1	LEU	A	179	63.840	48.212	11.998	1.00	42.26
ATOM	1298	CD2	LEU	A	179	66.122	47.176	12.048	1.00	44.90
ATOM	1299	C	LEU	A	179	65.226	45.669	16.108	1.00	46.31
ATOM	1300	O	LEU	A	179	66.243	45.936	16.747	1.00	45.30
ATOM	1301	N	TYR	A	180	64.070	45.389	16.690	1.00	44.68
ATOM	1302	CA	TYR	A	180	63.939	45.407	18.142	1.00	46.73
ATOM	1303	CB	TYR	A	180	62.482	45.175	18.568	1.00	45.38
ATOM	1304	CG	TYR	A	180	62.190	45.754	19.935	1.00	41.89
ATOM	1305	CD1	TYR	A	180	62.205	47.129	20.136	1.00	40.26
ATOM	1306	CE1	TYR	A	180	62.013	47.679	21.397	1.00	42.56
ATOM	1307	CD2	TYR	A	180	61.972	44.929	21.035	1.00	42.58
ATOM	1308	CE2	TYR	A	180	61.785	45.466	22.318	1.00	42.96
ATOM	1309	CZ	TYR	A	180	61.806	46.840	22.491	1.00	45.19
ATOM	1310	OH	TYR	A	180	61.638	47.378	23.749	1.00	43.42
ATOM	1311	C	TYR	A	180	64.837	44.398	18.851	1.00	45.62
ATOM	1312	O	TYR	A	180	65.384	44.702	19.900	1.00	42.68
ATOM	1313	N	GLU	A	181	64.981	43.204	18.281	1.00	47.80
ATOM	1314	CA	GLU	A	181	65.823	42.166	18.880	1.00	49.89
ATOM	1315	CB	GLU	A	181	65.702	40.847	18.102	1.00	50.32
ATOM	1316	CG	GLU	A	181	64.313	40.224	18.162	1.00	50.55
ATOM	1317	CD	GLU	A	181	64.177	38.988	17.289	1.00	52.58
ATOM	1318	OE1	GLU	A	181	65.134	38.668	16.550	1.00	53.64
ATOM	1319	OE2	GLU	A	181	63.107	38.340	17.337	1.00	52.87
ATOM	1320	C	GLU	A	181	67.277	42.615	18.901	1.00	50.81
ATOM	1321	O	GLU	A	181	67.954	42.506	19.922	1.00	51.41
ATOM	1322	N	GLU	A	182	67.762	43.121	17.775	1.00	50.01
ATOM	1323	CA	GLU	A	182	69.134	43.588	17.731	1.00	51.68
ATOM	1324	CB	GLU	A	182	69.485	44.065	16.322	1.00	54.11
ATOM	1325	CG	GLU	A	182	70.975	44.239	16.087	1.00	60.25
ATOM	1326	CD	GLU	A	182	71.293	44.660	14.665	1.00	66.17
ATOM	1327	OE1	GLU	A	182	72.477	44.958	14.383	1.00	68.16
ATOM	1328	OE2	GLU	A	182	70.359	44.688	13.831	1.00	69.10
ATOM	1329	C	GLU	A	182	69.261	44.728	18.749	1.00	49.69
ATOM	1330	O	GLU	A	182	70.240	44.806	19.482	1.00	53.34
ATOM	1331	N	TYR	A	183	68.246	45.586	18.810	1.00	47.99
ATOM	1332	CA	TYR	A	183	68.218	46.709	19.744	1.00	45.81
ATOM	1333	CB	TYR	A	183	66.928	47.499	19.542	1.00	42.49
ATOM	1334	CG	TYR	A	183	66.437	48.309	20.735	1.00	39.18
ATOM	1335	CD1	TYR	A	183	65.625	47.716	21.721	1.00	35.33
ATOM	1336	CE1	TYR	A	183	65.107	48.456	22.771	1.00	34.78
ATOM	1337	CD2	TYR	A	183	66.717	49.671	20.847	1.00	35.10
ATOM	1338	CE2	TYR	A	183	66.189	50.437	21.912	1.00	35.83
ATOM	1339	CZ	TYR	A	183	65.389	49.827	22.864	1.00	35.93
ATOM	1340	OH	TYR	A	183	64.837	50.566	23.906	1.00	35.91

125/396

Figure 2A-25

ATOM	1341	C	TYR	A	183	68.400	46.349	21.221	1.00	46.33
ATOM	1342	O	TYR	A	183	69.173	46.996	21.907	1.00	45.83
ATOM	1343	N	VAL	A	184	67.693	45.341	21.725	1.00	47.64
ATOM	1344	CA	VAL	A	184	67.867	44.972	23.127	1.00	50.89
ATOM	1345	CB	VAL	A	184	66.851	43.873	23.593	1.00	51.69
ATOM	1346	CG1	VAL	A	184	65.436	44.429	23.602	1.00	52.89
ATOM	1347	CG2	VAL	A	184	66.927	42.700	22.709	1.00	50.09
ATOM	1348	C	VAL	A	184	69.291	44.467	23.370	1.00	50.24
ATOM	1349	O	VAL	A	184	69.907	44.805	24.384	1.00	51.68
ATOM	1350	N	VAL	A	185	69.808	43.664	22.437	1.00	51.70
ATOM	1351	CA	VAL	A	185	71.171	43.131	22.535	1.00	52.32
ATOM	1352	CB	VAL	A	185	71.587	42.351	21.240	1.00	52.12
ATOM	1353	CG1	VAL	A	185	73.062	42.031	21.270	1.00	48.26
ATOM	1354	CG2	VAL	A	185	70.810	41.046	21.130	1.00	51.27
ATOM	1355	C	VAL	A	185	72.139	44.290	22.730	1.00	51.82
ATOM	1356	O	VAL	A	185	72.865	44.357	23.721	1.00	51.92
ATOM	1357	N	LEU	A	186	72.121	45.214	21.780	1.00	50.09
ATOM	1358	CA	LEU	A	186	72.990	46.375	21.820	1.00	49.54
ATOM	1359	CB	LEU	A	186	72.789	47.207	20.548	1.00	52.29
ATOM	1360	CG	LEU	A	186	73.833	47.087	19.433	1.00	55.31
ATOM	1361	CD1	LEU	A	186	74.480	45.712	19.421	1.00	56.69
ATOM	1362	CD2	LEU	A	186	73.154	47.381	18.106	1.00	56.79
ATOM	1363	C	LEU	A	186	72.804	47.253	23.046	1.00	47.73
ATOM	1364	O	LEU	A	186	73.771	47.808	23.565	1.00	49.89
ATOM	1365	N	LYS	A	187	71.570	47.382	23.510	1.00	46.80
ATOM	1366	CA	LYS	A	187	71.265	48.215	24.672	1.00	46.34
ATOM	1367	CB	LYS	A	187	69.765	48.519	24.713	1.00	48.71
ATOM	1368	CG	LYS	A	187	69.405	50.006	24.850	1.00	52.09
ATOM	1369	CD	LYS	A	187	69.940	50.823	23.702	1.00	48.22
ATOM	1370	CE	LYS	A	187	69.080	52.067	23.391	1.00	51.90
ATOM	1371	NZ	LYS	A	187	69.260	53.255	24.277	1.00	45.92
ATOM	1372	C	LYS	A	187	71.689	47.556	25.985	1.00	48.10
ATOM	1373	O	LYS	A	187	72.129	48.238	26.917	1.00	43.05
ATOM	1374	N	ASN	A	188	71.530	46.237	26.068	1.00	47.96
ATOM	1375	CA	ASN	A	188	71.925	45.522	27.272	1.00	52.05
ATOM	1376	CB	ASN	A	188	71.481	44.061	27.233	1.00	47.56
ATOM	1377	CG	ASN	A	188	70.131	43.852	27.870	1.00	50.47
ATOM	1378	OD1	ASN	A	188	69.721	44.614	28.758	1.00	47.37
ATOM	1379	ND2	ASN	A	188	69.434	42.801	27.444	1.00	50.28
ATOM	1380	C	ASN	A	188	73.436	45.580	27.373	1.00	54.02
ATOM	1381	O	ASN	A	188	74.002	45.586	28.466	1.00	56.22
ATOM	1382	N	GLU	A	189	74.081	45.632	26.217	1.00	55.62
ATOM	1383	CA	GLU	A	189	75.530	45.698	26.155	1.00	58.73
ATOM	1384	CB	GLU	A	189	75.976	45.496	24.711	1.00	63.17
ATOM	1385	CG	GLU	A	189	77.391	45.025	24.548	1.00	68.50
ATOM	1386	CD	GLU	A	189	77.634	44.469	23.164	1.00	73.35
ATOM	1387	OE1	GLU	A	189	76.843	43.595	22.735	1.00	73.12
ATOM	1388	OE2	GLU	A	189	78.614	44.899	22.509	1.00	76.92
ATOM	1389	C	GLU	A	189	75.971	47.063	26.668	1.00	58.25
ATOM	1390	O	GLU	A	189	76.896	47.166	27.455	1.00	58.72
ATOM	1391	N	MET	A	190	75.297	48.118	26.221	1.00	58.21
ATOM	1392	CA	MET	A	190	75.631	49.453	26.674	1.00	56.16
ATOM	1393	CB	MET	A	190	74.701	50.494	26.030	1.00	59.05
ATOM	1394	CG	MET	A	190	74.759	51.892	26.648	1.00	56.16
ATOM	1395	SD	MET	A	190	73.342	52.245	27.738	1.00	67.23
ATOM	1396	CE	MET	A	190	74.069	52.267	29.321	1.00	61.32

126/396

Figure 2A-26

ATOM	1397	C	MET	A	190	75.478	49.470	28.182	1.00	55.45
ATOM	1398	O	MET	A	190	76.402	49.854	28.904	1.00	57.97
ATOM	1399	N	ALA	A	191	74.318	49.022	28.650	1.00	51.62
ATOM	1400	CA	ALA	A	191	74.004	48.995	30.072	1.00	51.01
ATOM	1401	CB	ALA	A	191	72.602	48.444	30.267	1.00	45.52
ATOM	1402	C	ALA	A	191	75.011	48.217	30.947	1.00	53.54
ATOM	1403	O	ALA	A	191	75.427	48.696	32.004	1.00	52.74
ATOM	1404	N	ARG	A	192	75.401	47.025	30.515	1.00	55.26
ATOM	1405	CA	ARG	A	192	76.350	46.227	31.286	1.00	57.99
ATOM	1406	CB	ARG	A	192	76.560	44.853	30.641	1.00	56.86
ATOM	1407	CG	ARG	A	192	75.380	43.899	30.785	1.00	56.30
ATOM	1408	CD	ARG	A	192	75.813	42.468	30.507	1.00	55.23
ATOM	1409	NE	ARG	A	192	76.303	42.288	29.141	1.00	57.55
ATOM	1410	CZ	ARG	A	192	75.515	42.082	28.088	1.00	59.93
ATOM	1411	NH1	ARG	A	192	76.038	41.932	26.879	1.00	60.13
ATOM	1412	NH2	ARG	A	192	74.200	42.015	28.245	1.00	59.02
ATOM	1413	C	ARG	A	192	77.692	46.949	31.406	1.00	58.27
ATOM	1414	O	ARG	A	192	78.225	47.114	32.506	1.00	58.91
ATOM	1415	N	ALA	A	193	78.222	47.394	30.271	1.00	57.92
ATOM	1416	CA	ALA	A	193	79.495	48.093	30.248	1.00	57.65
ATOM	1417	CB	ALA	A	193	79.872	48.427	28.831	1.00	57.50
ATOM	1418	C	ALA	A	193	79.451	49.358	31.087	1.00	59.57
ATOM	1419	O	ALA	A	193	80.489	49.941	31.390	1.00	61.70
ATOM	1420	N	ASN	A	194	78.245	49.778	31.454	1.00	61.01
ATOM	1421	CA	ASN	A	194	78.037	50.975	32.270	1.00	59.94
ATOM	1422	CB	ASN	A	194	76.836	51.768	31.748	1.00	62.95
ATOM	1423	CG	ASN	A	194	77.223	52.786	30.698	1.00	64.57
ATOM	1424	OD1	ASN	A	194	77.797	53.829	31.013	1.00	68.07
ATOM	1425	ND2	ASN	A	194	76.920	52.487	29.441	1.00	63.82
ATOM	1426	C	ASN	A	194	77.796	50.574	33.717	1.00	58.83
ATOM	1427	O	ASN	A	194	77.384	51.390	34.544	1.00	58.27
ATOM	1428	N	HIS	A	195	78.031	49.297	33.996	1.00	58.25
ATOM	1429	CA	HIS	A	195	77.896	48.735	35.332	1.00	59.03
ATOM	1430	CB	HIS	A	195	78.725	49.578	36.317	1.00	60.21
ATOM	1431	CG	HIS	A	195	80.117	49.837	35.830	1.00	62.48
ATOM	1432	CD2	HIS	A	195	81.071	48.984	35.382	1.00	61.95
ATOM	1433	ND1	HIS	A	195	80.602	51.109	35.601	1.00	62.59
ATOM	1434	CE1	HIS	A	195	81.786	51.028	35.021	1.00	62.93
ATOM	1435	NE2	HIS	A	195	82.093	49.750	34.875	1.00	63.67
ATOM	1436	C	HIS	A	195	76.471	48.527	35.833	1.00	58.30
ATOM	1437	O	HIS	A	195	76.170	48.714	37.017	1.00	60.69
ATOM	1438	N	TYR	A	196	75.596	48.132	34.918	1.00	55.51
ATOM	1439	CA	TYR	A	196	74.213	47.831	35.250	1.00	52.31
ATOM	1440	CB	TYR	A	196	73.251	48.792	34.534	1.00	54.28
ATOM	1441	CG	TYR	A	196	73.258	50.215	35.054	1.00	50.51
ATOM	1442	CD1	TYR	A	196	72.465	50.587	36.142	1.00	47.23
ATOM	1443	CE1	TYR	A	196	72.463	51.899	36.618	1.00	49.14
ATOM	1444	CD2	TYR	A	196	74.054	51.190	34.451	1.00	45.75
ATOM	1445	CE2	TYR	A	196	74.064	52.496	34.917	1.00	48.31
ATOM	1446	CZ	TYR	A	196	73.269	52.848	35.998	1.00	51.08
ATOM	1447	OH	TYR	A	196	73.292	54.145	36.451	1.00	51.04
ATOM	1448	C	TYR	A	196	73.971	46.405	34.760	1.00	51.05
ATOM	1449	O	TYR	A	196	74.686	45.906	33.884	1.00	48.70
ATOM	1450	N	GLU	A	197	72.961	45.751	35.319	1.00	53.69
ATOM	1451	CA	GLU	A	197	72.617	44.380	34.926	1.00	55.09
ATOM	1452	CB	GLU	A	197	71.552	43.826	35.868	1.00	56.57

127/396

Figure 2A-27

ATOM	1453	CG	GLU	A	197	71.948	43.828	37.326	1.00	59.59
ATOM	1454	CD	GLU	A	197	70.749	43.902	38.239	1.00	63.97
ATOM	1455	OE1	GLU	A	197	69.759	43.164	38.002	1.00	63.96
ATOM	1456	OE2	GLU	A	197	70.801	44.705	39.195	1.00	64.20
ATOM	1457	C	GLU	A	197	72.081	44.308	33.496	1.00	55.74
ATOM	1458	O	GLU	A	197	72.480	43.448	32.704	1.00	55.85
ATOM	1459	N	ASP	A	198	71.155	45.208	33.184	1.00	55.88
ATOM	1460	CA	ASP	A	198	70.531	45.260	31.868	1.00	56.15
ATOM	1461	CB	ASP	A	198	69.435	44.198	31.769	1.00	57.63
ATOM	1462	CG	ASP	A	198	68.485	44.237	32.946	1.00	62.55
ATOM	1463	OD1	ASP	A	198	68.477	43.262	33.731	1.00	63.52
ATOM	1464	OD2	ASP	A	198	67.749	45.244	33.092	1.00	64.91
ATOM	1465	C	ASP	A	198	69.936	46.645	31.614	1.00	54.81
ATOM	1466	O	ASP	A	198	69.849	47.477	32.525	1.00	52.10
ATOM	1467	N	TYR	A	199	69.502	46.875	30.378	1.00	53.19
ATOM	1468	CA	TYR	A	199	68.950	48.173	29.999	1.00	50.17
ATOM	1469	CB	TYR	A	199	68.525	48.143	28.530	1.00	49.04
ATOM	1470	CG	TYR	A	199	68.174	49.503	27.965	1.00	51.41
ATOM	1471	CD1	TYR	A	199	68.970	50.614	28.230	1.00	52.48
ATOM	1472	CE1	TYR	A	199	68.675	51.850	27.684	1.00	53.99
ATOM	1473	CD2	TYR	A	199	67.065	49.667	27.138	1.00	52.35
ATOM	1474	CE2	TYR	A	199	66.760	50.894	26.583	1.00	51.88
ATOM	1475	CZ	TYR	A	199	67.566	51.979	26.856	1.00	55.42
ATOM	1476	OH	TYR	A	199	67.289	53.179	26.274	1.00	53.61
ATOM	1477	C	TYR	A	199	67.801	48.628	30.905	1.00	48.45
ATOM	1478	O	TYR	A	199	67.691	49.811	31.227	1.00	45.37
ATOM	1479	N	GLY	A	200	66.970	47.687	31.344	1.00	46.50
ATOM	1480	CA	GLY	A	200	65.875	48.043	32.223	1.00	44.30
ATOM	1481	C	GLY	A	200	66.350	48.463	33.605	1.00	46.66
ATOM	1482	O	GLY	A	200	65.748	49.326	34.249	1.00	44.24
ATOM	1483	N	ASP	A	201	67.416	47.827	34.084	1.00	47.39
ATOM	1484	CA	ASP	A	201	67.981	48.164	35.386	1.00	46.10
ATOM	1485	CB	ASP	A	201	69.103	47.154	35.727	1.00	49.12
ATOM	1486	CG	ASP	A	201	69.841	47.490	37.018	1.00	50.70
ATOM	1487	OD1	ASP	A	201	69.194	47.699	38.070	1.00	53.26
ATOM	1488	OD2	ASP	A	201	71.084	47.542	36.976	1.00	59.31
ATOM	1489	C	ASP	A	201	68.528	49.598	35.243	1.00	43.42
ATOM	1490	O	ASP	A	201	68.441	50.411	36.151	1.00	39.63
ATOM	1491	N	TYR	A	202	69.085	49.882	34.073	1.00	45.92
ATOM	1492	CA	TYR	A	202	69.624	51.198	33.737	1.00	48.98
ATOM	1493	CB	TYR	A	202	70.113	51.170	32.282	1.00	53.01
ATOM	1494	CG	TYR	A	202	70.711	52.462	31.758	1.00	56.08
ATOM	1495	CD1	TYR	A	202	72.010	52.848	32.108	1.00	60.31
ATOM	1496	CE1	TYR	A	202	72.585	54.015	31.589	1.00	61.16
ATOM	1497	CD2	TYR	A	202	69.991	53.280	30.880	1.00	55.72
ATOM	1498	CE2	TYR	A	202	70.544	54.445	30.355	1.00	57.96
ATOM	1499	CZ	TYR	A	202	71.846	54.807	30.708	1.00	63.92
ATOM	1500	OH	TYR	A	202	72.421	55.929	30.145	1.00	67.25
ATOM	1501	C	TYR	A	202	68.548	52.287	33.917	1.00	48.20
ATOM	1502	O	TYR	A	202	68.806	53.329	34.524	1.00	50.15
ATOM	1503	N	TRP	A	203	67.343	52.042	33.399	1.00	44.50
ATOM	1504	CA	TRP	A	203	66.239	53.001	33.512	1.00	43.03
ATOM	1505	CB	TRP	A	203	65.020	52.538	32.684	1.00	44.01
ATOM	1506	CG	TRP	A	203	65.109	52.786	31.206	1.00	47.42
ATOM	1507	CD2	TRP	A	203	64.290	52.195	30.191	1.00	44.11
ATOM	1508	CE2	TRP	A	203	64.703	52.734	28.956	1.00	44.72

128/396

Figure 2A-28

ATOM	1509	CE3	TRP	A	203	63.244	51.260	30.208	1.00	47.92
ATOM	1510	CD1	TRP	A	203	65.960	53.643	30.561	1.00	48.18
ATOM	1511	NE1	TRP	A	203	65.722	53.615	29.211	1.00	45.67
ATOM	1512	CZ2	TRP	A	203	64.107	52.368	27.740	1.00	46.07
ATOM	1513	CZ3	TRP	A	203	62.650	50.893	28.999	1.00	45.49
ATOM	1514	CH2	TRP	A	203	63.088	51.449	27.782	1.00	46.09
ATOM	1515	C	TRP	A	203	65.763	53.231	34.942	1.00	41.80
ATOM	1516	O	TRP	A	203	65.409	54.357	35.324	1.00	40.44
ATOM	1517	N	ARG	A	204	65.685	52.152	35.715	1.00	41.66
ATOM	1518	CA	ARG	A	204	65.241	52.255	37.093	1.00	43.90
ATOM	1519	CB	ARG	A	204	65.076	50.855	37.705	1.00	45.78
ATOM	1520	CG	ARG	A	204	63.979	50.021	37.035	1.00	44.48
ATOM	1521	CD	ARG	A	204	63.703	48.703	37.775	1.00	47.40
ATOM	1522	NE	ARG	A	204	64.813	47.747	37.720	1.00	40.96
ATOM	1523	CZ	ARG	A	204	64.983	46.842	36.758	1.00	48.32
ATOM	1524	NH1	ARG	A	204	64.119	46.762	35.752	1.00	51.38
ATOM	1525	NH2	ARG	A	204	66.001	45.988	36.811	1.00	48.18
ATOM	1526	C	ARG	A	204	66.267	53.095	37.858	1.00	44.76
ATOM	1527	O	ARG	A	204	66.022	53.554	38.969	1.00	45.53
ATOM	1528	N	GLY	A	205	67.412	53.305	37.225	1.00	46.96
ATOM	1529	CA	GLY	A	205	68.454	54.123	37.806	1.00	48.17
ATOM	1530	C	GLY	A	205	67.982	55.538	38.116	1.00	50.93
ATOM	1531	O	GLY	A	205	68.653	56.245	38.885	1.00	49.42
ATOM	1532	N	ASP	A	206	66.843	55.962	37.548	1.00	48.76
ATOM	1533	CA	ASP	A	206	66.328	57.325	37.807	1.00	48.38
ATOM	1534	CB	ASP	A	206	65.238	57.722	36.802	1.00	48.13
ATOM	1535	CG	ASP	A	206	64.742	59.159	37.003	1.00	48.53
ATOM	1536	OD1	ASP	A	206	63.705	59.364	37.678	1.00	45.64
ATOM	1537	OD2	ASP	A	206	65.401	60.095	36.487	1.00	48.75
ATOM	1538	C	ASP	A	206	65.759	57.502	39.205	1.00	48.46
ATOM	1539	O	ASP	A	206	65.673	58.628	39.697	1.00	48.14
ATOM	1540	N	TYR	A	207	65.356	56.399	39.837	1.00	47.64
ATOM	1541	CA	TYR	A	207	64.792	56.457	41.181	1.00	48.31
ATOM	1542	CB	TYR	A	207	63.609	55.498	41.283	1.00	48.75
ATOM	1543	CG	TYR	A	207	62.518	55.778	40.275	1.00	48.71
ATOM	1544	CD1	TYR	A	207	62.560	55.224	38.993	1.00	50.72
ATOM	1545	CE1	TYR	A	207	61.568	55.515	38.052	1.00	53.68
ATOM	1546	CD2	TYR	A	207	61.463	56.622	40.596	1.00	48.42
ATOM	1547	CE2	TYR	A	207	60.468	56.919	39.674	1.00	52.07
ATOM	1548	CZ	TYR	A	207	60.526	56.365	38.406	1.00	52.40
ATOM	1549	OH	TYR	A	207	59.533	56.668	37.504	1.00	55.28
ATOM	1550	C	TYR	A	207	65.821	56.135	42.296	1.00	48.76
ATOM	1551	O	TYR	A	207	65.557	56.333	43.487	1.00	43.57
ATOM	1552	N	GLU	A	208	66.991	55.661	41.898	1.00	47.90
ATOM	1553	CA	GLU	A	208	68.026	55.309	42.852	1.00	53.85
ATOM	1554	CB	GLU	A	208	69.129	54.507	42.161	1.00	51.16
ATOM	1555	CG	GLU	A	208	70.348	54.301	43.027	1.00	55.50
ATOM	1556	CD	GLU	A	208	71.353	53.349	42.419	1.00	59.80
ATOM	1557	OE1	GLU	A	208	71.587	53.411	41.185	1.00	61.13
ATOM	1558	OE2	GLU	A	208	71.924	52.541	43.184	1.00	65.40
ATOM	1559	C	GLU	A	208	68.652	56.484	43.586	1.00	56.87
ATOM	1560	O	GLU	A	208	69.037	57.482	42.981	1.00	59.99
ATOM	1561	N	VAL	A	209	68.739	56.359	44.902	1.00	57.96
ATOM	1562	CA	VAL	A	209	69.358	57.384	45.715	1.00	62.84
ATOM	1563	CB	VAL	A	209	68.299	58.316	46.352	1.00	63.03
ATOM	1564	CG1	VAL	A	209	66.939	57.678	46.274	1.00	63.56

129/396

Figure 2A-29

ATOM	1565	CG2	VAL	A	209	68.681	58.649	47.799	1.00	59.63
ATOM	1566	C	VAL	A	209	70.205	56.675	46.774	1.00	65.00
ATOM	1567	O	VAL	A	209	69.733	55.746	47.441	1.00	64.66
ATOM	1568	N	ASN	A	210	71.461	57.100	46.901	1.00	65.91
ATOM	1569	CA	ASN	A	210	72.394	56.490	47.846	1.00	67.05
ATOM	1570	CB	ASN	A	210	73.398	55.635	47.081	1.00	67.02
ATOM	1571	CG	ASN	A	210	72.743	54.457	46.390	1.00	71.67
ATOM	1572	OD1	ASN	A	210	73.393	53.701	45.669	1.00	73.10
ATOM	1573	ND2	ASN	A	210	71.442	54.293	46.610	1.00	72.68
ATOM	1574	C	ASN	A	210	73.160	57.460	48.739	1.00	68.34
ATOM	1575	O	ASN	A	210	73.088	58.686	48.575	1.00	66.92
ATOM	1576	N	GLY	A	211	73.899	56.887	49.688	1.00	68.10
ATOM	1577	CA	GLY	A	211	74.700	57.684	50.603	1.00	67.70
ATOM	1578	C	GLY	A	211	73.915	58.698	51.406	1.00	67.61
ATOM	1579	O	GLY	A	211	74.436	59.748	51.776	1.00	69.66
ATOM	1580	N	VAL	A	212	72.650	58.395	51.664	1.00	68.07
ATOM	1581	CA	VAL	A	212	71.797	59.280	52.445	1.00	68.14
ATOM	1582	CB	VAL	A	212	70.882	60.139	51.551	1.00	66.08
ATOM	1583	CG1	VAL	A	212	70.067	61.095	52.411	1.00	65.41
ATOM	1584	CG2	VAL	A	212	71.715	60.910	50.543	1.00	65.88
ATOM	1585	C	VAL	A	212	70.940	58.391	53.332	1.00	70.38
ATOM	1586	O	VAL	A	212	69.953	57.818	52.884	1.00	71.41
ATOM	1587	N	ASP	A	213	71.335	58.281	54.595	1.00	71.82
ATOM	1588	CA	ASP	A	213	70.640	57.447	55.568	1.00	71.98
ATOM	1589	CB	ASP	A	213	71.404	57.496	56.891	1.00	76.04
ATOM	1590	CG	ASP	A	213	72.886	57.222	56.709	1.00	81.52
ATOM	1591	OD1	ASP	A	213	73.345	56.125	57.108	1.00	81.89
ATOM	1592	OD2	ASP	A	213	73.586	58.105	56.150	1.00	83.22
ATOM	1593	C	ASP	A	213	69.181	57.843	55.793	1.00	68.74
ATOM	1594	O	ASP	A	213	68.878	58.987	56.137	1.00	68.80
ATOM	1595	N	GLY	A	214	68.278	56.887	55.601	1.00	66.61
ATOM	1596	CA	GLY	A	214	66.868	57.161	55.800	1.00	65.64
ATOM	1597	C	GLY	A	214	66.095	57.528	54.541	1.00	64.79
ATOM	1598	O	GLY	A	214	64.875	57.674	54.587	1.00	64.97
ATOM	1599	N	TYR	A	215	66.789	57.677	53.418	1.00	61.18
ATOM	1600	CA	TYR	A	215	66.124	58.036	52.174	1.00	60.07
ATOM	1601	CB	TYR	A	215	66.271	59.533	51.913	1.00	55.45
ATOM	1602	CG	TYR	A	215	65.634	60.394	52.970	1.00	55.79
ATOM	1603	CD1	TYR	A	215	64.257	60.608	52.992	1.00	53.95
ATOM	1604	CE1	TYR	A	215	63.670	61.421	53.967	1.00	58.04
ATOM	1605	CD2	TYR	A	215	66.416	61.013	53.959	1.00	60.82
ATOM	1606	CE2	TYR	A	215	65.838	61.831	54.944	1.00	55.18
ATOM	1607	CZ	TYR	A	215	64.474	62.030	54.937	1.00	58.40
ATOM	1608	OH	TYR	A	215	63.919	62.862	55.874	1.00	60.68
ATOM	1609	C	TYR	A	215	66.682	57.260	50.994	1.00	59.16
ATOM	1610	O	TYR	A	215	66.337	57.542	49.847	1.00	62.63
ATOM	1611	N	ASP	A	216	67.550	56.291	51.269	1.00	56.59
ATOM	1612	CA	ASP	A	216	68.127	55.487	50.204	1.00	56.96
ATOM	1613	CB	ASP	A	216	69.194	54.543	50.756	1.00	57.45
ATOM	1614	CG	ASP	A	216	70.545	55.220	50.902	1.00	62.24
ATOM	1615	OD1	ASP	A	216	71.531	54.542	51.267	1.00	67.76
ATOM	1616	OD2	ASP	A	216	70.624	56.436	50.645	1.00	63.67
ATOM	1617	C	ASP	A	216	67.040	54.693	49.477	1.00	54.19
ATOM	1618	O	ASP	A	216	65.973	54.434	50.026	1.00	54.36
ATOM	1619	N	TYR	A	217	67.313	54.311	48.239	1.00	50.61
ATOM	1620	CA	TYR	A	217	66.330	53.584	47.462	1.00	48.71

130/396

Figure 2A-30

ATOM	1621	CB	TYR	A	217	65.339	54.575	46.832	1.00	50.26
ATOM	1622	CG	TYR	A	217	64.087	53.924	46.285	1.00	46.81
ATOM	1623	CD1	TYR	A	217	62.967	53.742	47.085	1.00	46.47
ATOM	1624	CE1	TYR	A	217	61.827	53.109	46.590	1.00	48.86
ATOM	1625	CD2	TYR	A	217	64.042	53.460	44.977	1.00	47.17
ATOM	1626	CE2	TYR	A	217	62.912	52.823	44.476	1.00	49.72
ATOM	1627	CZ	TYR	A	217	61.811	52.651	45.284	1.00	48.01
ATOM	1628	OH	TYR	A	217	60.704	52.003	44.775	1.00	48.27
ATOM	1629	C	TYR	A	217	67.020	52.777	46.386	1.00	45.56
ATOM	1630	O	TYR	A	217	67.801	53.296	45.597	1.00	48.68
ATOM	1631	N	SER	A	218	66.712	51.496	46.347	1.00	46.96
ATOM	1632	CA	SER	A	218	67.322	50.589	45.388	1.00	49.17
ATOM	1633	CB	SER	A	218	67.322	49.174	45.979	1.00	45.38
ATOM	1634	OG	SER	A	218	67.802	48.231	45.033	1.00	56.05
ATOM	1635	C	SER	A	218	66.621	50.575	44.020	1.00	47.56
ATOM	1636	O	SER	A	218	65.453	50.940	43.908	1.00	49.03
ATOM	1637	N	ARG	A	219	67.340	50.133	42.993	1.00	47.92
ATOM	1638	CA	ARG	A	219	66.777	50.056	41.653	1.00	52.45
ATOM	1639	CB	ARG	A	219	67.881	49.828	40.608	1.00	47.52
ATOM	1640	CG	ARG	A	219	68.871	50.965	40.515	1.00	47.56
ATOM	1641	CD	ARG	A	219	69.584	50.987	39.182	1.00	49.79
ATOM	1642	NE	ARG	A	219	70.592	49.939	39.040	1.00	53.98
ATOM	1643	CZ	ARG	A	219	71.842	50.033	39.494	1.00	52.82
ATOM	1644	NH1	ARG	A	219	72.256	51.128	40.127	1.00	48.20
ATOM	1645	NH2	ARG	A	219	72.685	49.032	39.299	1.00	49.25
ATOM	1646	C	ARG	A	219	65.753	48.923	41.590	1.00	55.47
ATOM	1647	O	ARG	A	219	64.708	49.057	40.940	1.00	56.42
ATOM	1648	N	GLY	A	220	66.057	47.813	42.269	1.00	55.18
ATOM	1649	CA	GLY	A	220	65.151	46.670	42.300	1.00	51.47
ATOM	1650	C	GLY	A	220	63.958	46.954	43.189	1.00	50.71
ATOM	1651	O	GLY	A	220	62.892	46.357	43.046	1.00	52.33
ATOM	1652	N	GLN	A	221	64.140	47.885	44.115	1.00	49.02
ATOM	1653	CA	GLN	A	221	63.089	48.278	45.041	1.00	49.04
ATOM	1654	CB	GLN	A	221	63.670	49.276	46.047	1.00	50.58
ATOM	1655	CG	GLN	A	221	62.833	49.551	47.273	1.00	56.70
ATOM	1656	CD	GLN	A	221	63.605	50.333	48.335	1.00	66.46
ATOM	1657	OE1	GLN	A	221	64.806	50.103	48.556	1.00	67.64
ATOM	1658	NE2	GLN	A	221	62.916	51.249	49.010	1.00	69.31
ATOM	1659	C	GLN	A	221	61.912	48.908	44.276	1.00	49.78
ATOM	1660	O	GLN	A	221	60.776	48.884	44.749	1.00	47.44
ATOM	1661	N	LEU	A	222	62.196	49.490	43.106	1.00	50.86
ATOM	1662	CA	LEU	A	222	61.160	50.107	42.272	1.00	45.58
ATOM	1663	CB	LEU	A	222	61.771	50.766	41.025	1.00	47.09
ATOM	1664	CG	LEU	A	222	60.761	51.401	40.052	1.00	45.14
ATOM	1665	CD1	LEU	A	222	60.103	52.618	40.707	1.00	48.32
ATOM	1666	CD2	LEU	A	222	61.463	51.816	38.776	1.00	51.63
ATOM	1667	C	LEU	A	222	60.193	49.027	41.819	1.00	43.05
ATOM	1668	O	LEU	A	222	58.984	49.173	41.915	1.00	41.25
ATOM	1669	N	ILE	A	223	60.737	47.934	41.314	1.00	45.90
ATOM	1670	CA	ILE	A	223	59.898	46.845	40.845	1.00	49.29
ATOM	1671	CB	ILE	A	223	60.719	45.630	40.374	1.00	48.44
ATOM	1672	CG2	ILE	A	223	59.771	44.566	39.822	1.00	47.03
ATOM	1673	CG1	ILE	A	223	61.737	46.054	39.320	1.00	46.56
ATOM	1674	CD1	ILE	A	223	62.553	44.908	38.743	1.00	47.47
ATOM	1675	C	ILE	A	223	58.931	46.341	41.899	1.00	51.57
ATOM	1676	O	ILE	A	223	57.797	46.006	41.568	1.00	57.48

131/396

Figure 2A-31

ATOM	1677	N	GLU	A	224	59.344	46.275	43.162	1.00	51.60
ATOM	1678	CA	GLU	A	224	58.420	45.764	44.171	1.00	53.33
ATOM	1679	CB	GLU	A	224	59.171	45.036	45.313	1.00	58.30
ATOM	1680	CG	GLU	A	224	60.135	45.856	46.156	1.00	65.86
ATOM	1681	CD	GLU	A	224	61.036	44.979	47.040	1.00	70.63
ATOM	1682	OE1	GLU	A	224	61.845	44.204	46.480	1.00	71.68
ATOM	1683	OE2	GLU	A	224	60.940	45.063	48.290	1.00	71.28
ATOM	1684	C	GLU	A	224	57.438	46.793	44.718	1.00	50.48
ATOM	1685	O	GLU	A	224	56.333	46.437	45.126	1.00	47.75
ATOM	1686	N	ASP	A	225	57.807	48.068	44.720	1.00	49.23
ATOM	1687	CA	ASP	A	225	56.864	49.071	45.201	1.00	48.00
ATOM	1688	CB	ASP	A	225	57.583	50.382	45.493	1.00	51.96
ATOM	1689	CG	ASP	A	225	58.570	50.241	46.629	1.00	57.99
ATOM	1690	OD1	ASP	A	225	58.282	49.448	47.553	1.00	60.28
ATOM	1691	OD2	ASP	A	225	59.614	50.915	46.608	1.00	60.97
ATOM	1692	C	ASP	A	225	55.770	49.272	44.154	1.00	47.34
ATOM	1693	O	ASP	A	225	54.628	49.601	44.486	1.00	43.91
ATOM	1694	N	VAL	A	226	56.130	49.062	42.889	1.00	45.48
ATOM	1695	CA	VAL	A	226	55.174	49.186	41.796	1.00	47.23
ATOM	1696	CB	VAL	A	226	55.910	49.177	40.393	1.00	44.74
ATOM	1697	CG1	VAL	A	226	54.928	48.891	39.273	1.00	45.76
ATOM	1698	CG2	VAL	A	226	56.569	50.543	40.141	1.00	44.12
ATOM	1699	C	VAL	A	226	54.189	48.015	41.923	1.00	43.76
ATOM	1700	O	VAL	A	226	52.978	48.205	42.010	1.00	45.63
ATOM	1701	N	GLU	A	227	54.713	46.802	41.970	1.00	47.51
ATOM	1702	CA	GLU	A	227	53.861	45.621	42.091	1.00	48.03
ATOM	1703	CB	GLU	A	227	54.718	44.367	41.991	1.00	50.20
ATOM	1704	CG	GLU	A	227	55.549	44.391	40.724	1.00	53.48
ATOM	1705	CD	GLU	A	227	56.331	43.128	40.488	1.00	57.88
ATOM	1706	OE1	GLU	A	227	56.841	42.555	41.478	1.00	60.89
ATOM	1707	OE2	GLU	A	227	56.454	42.725	39.306	1.00	53.96
ATOM	1708	C	GLU	A	227	53.026	45.606	43.358	1.00	47.82
ATOM	1709	O	GLU	A	227	51.891	45.147	43.338	1.00	49.85
ATOM	1710	N	HIS	A	228	53.567	46.131	44.453	1.00	47.40
ATOM	1711	CA	HIS	A	228	52.832	46.164	45.717	1.00	49.74
ATOM	1712	CB	HIS	A	228	53.779	46.502	46.887	1.00	50.90
ATOM	1713	CG	HIS	A	228	53.074	46.776	48.180	1.00	55.16
ATOM	1714	CD2	HIS	A	228	52.877	45.998	49.272	1.00	59.82
ATOM	1715	ND1	HIS	A	228	52.444	47.975	48.447	1.00	60.91
ATOM	1716	CE1	HIS	A	228	51.889	47.923	49.647	1.00	60.70
ATOM	1717	NE2	HIS	A	228	52.137	46.733	50.169	1.00	58.74
ATOM	1718	C	HIS	A	228	51.702	47.176	45.642	1.00	49.15
ATOM	1719	O	HIS	A	228	50.584	46.917	46.095	1.00	51.76
ATOM	1720	N	THR	A	229	51.989	48.337	45.075	1.00	46.95
ATOM	1721	CA	THR	A	229	50.961	49.360	44.936	1.00	46.40
ATOM	1722	CB	THR	A	229	51.588	50.713	44.530	1.00	47.46
ATOM	1723	OG1	THR	A	229	50.542	51.667	44.340	1.00	58.67
ATOM	1724	CG2	THR	A	229	52.395	50.581	43.232	1.00	36.74
ATOM	1725	C	THR	A	229	49.915	48.935	43.879	1.00	42.86
ATOM	1726	O	THR	A	229	48.731	49.237	43.999	1.00	42.22
ATOM	1727	N	PHE	A	230	50.354	48.217	42.854	1.00	44.20
ATOM	1728	CA	PHE	A	230	49.444	47.771	41.810	1.00	47.11
ATOM	1729	CB	PHE	A	230	50.227	47.116	40.670	1.00	48.22
ATOM	1730	CG	PHE	A	230	49.365	46.710	39.526	1.00	49.66
ATOM	1731	CD1	PHE	A	230	48.647	47.668	38.816	1.00	48.68
ATOM	1732	CD2	PHE	A	230	49.188	45.363	39.214	1.00	50.73

132/396

Figure 2A-32

ATOM	1733	CE1	PHE	A	230	47.757	47.298	37.815	1.00	48.59
ATOM	1734	CE2	PHE	A	230	48.293	44.979	38.211	1.00	51.00
ATOM	1735	CZ	PHE	A	230	47.577	45.948	37.513	1.00	50.24
ATOM	1736	C	PHE	A	230	48.383	46.805	42.368	1.00	49.48
ATOM	1737	O	PHE	A	230	47.207	46.873	41.984	1.00	46.90
ATOM	1738	N	GLU	A	231	48.795	45.924	43.285	1.00	51.66
ATOM	1739	CA	GLU	A	231	47.876	44.970	43.919	1.00	52.72
ATOM	1740	CB	GLU	A	231	48.585	44.158	45.003	1.00	55.78
ATOM	1741	CG	GLU	A	231	49.464	43.030	44.490	1.00	65.44
ATOM	1742	CD	GLU	A	231	48.665	41.915	43.834	1.00	69.99
ATOM	1743	OE1	GLU	A	231	47.615	41.531	44.400	1.00	73.04
ATOM	1744	OE2	GLU	A	231	49.094	41.417	42.766	1.00	72.74
ATOM	1745	C	GLU	A	231	46.703	45.688	44.553	1.00	50.43
ATOM	1746	O	GLU	A	231	45.562	45.250	44.436	1.00	51.52
ATOM	1747	N	GLU	A	232	46.986	46.789	45.235	1.00	48.80
ATOM	1748	CA	GLU	A	232	45.934	47.569	45.882	1.00	50.62
ATOM	1749	CB	GLU	A	232	46.553	48.640	46.785	1.00	54.96
ATOM	1750	CG	GLU	A	232	46.809	48.190	48.214	1.00	64.24
ATOM	1751	CD	GLU	A	232	47.561	49.227	49.026	1.00	66.71
ATOM	1752	OE1	GLU	A	232	48.780	49.399	48.783	1.00	71.89
ATOM	1753	OE2	GLU	A	232	46.934	49.870	49.896	1.00	65.96
ATOM	1754	C	GLU	A	232	44.993	48.251	44.897	1.00	48.88
ATOM	1755	O	GLU	A	232	43.889	48.637	45.258	1.00	50.64
ATOM	1756	N	ILE	A	233	45.438	48.412	43.658	1.00	48.93
ATOM	1757	CA	ILE	A	233	44.630	49.074	42.641	1.00	51.26
ATOM	1758	CB	ILE	A	233	45.562	49.809	41.622	1.00	52.94
ATOM	1759	CG2	ILE	A	233	45.726	48.991	40.364	1.00	56.11
ATOM	1760	CG1	ILE	A	233	44.987	51.172	41.266	1.00	54.98
ATOM	1761	CD1	ILE	A	233	43.718	51.104	40.453	1.00	57.59
ATOM	1762	C	ILE	A	233	43.710	48.084	41.915	1.00	49.16
ATOM	1763	O	ILE	A	233	42.670	48.461	41.389	1.00	49.05
ATOM	1764	N	LYS	A	234	44.095	46.814	41.913	1.00	50.96
ATOM	1765	CA	LYS	A	234	43.324	45.770	41.241	1.00	53.74
ATOM	1766	CB	LYS	A	234	43.910	44.387	41.550	1.00	52.36
ATOM	1767	CG	LYS	A	234	45.167	44.047	40.756	1.00	56.00
ATOM	1768	CD	LYS	A	234	45.671	42.620	41.068	1.00	56.82
ATOM	1769	CE	LYS	A	234	46.938	42.287	40.285	1.00	60.63
ATOM	1770	NZ	LYS	A	234	47.534	40.953	40.615	1.00	62.35
ATOM	1771	C	LYS	A	234	41.810	45.734	41.466	1.00	52.82
ATOM	1772	O	LYS	A	234	41.060	45.632	40.504	1.00	54.39
ATOM	1773	N	PRO	A	235	41.337	45.807	42.726	1.00	52.37
ATOM	1774	CD	PRO	A	235	42.042	45.785	44.023	1.00	54.95
ATOM	1775	CA	PRO	A	235	39.885	45.770	42.927	1.00	50.54
ATOM	1776	CB	PRO	A	235	39.738	45.884	44.449	1.00	51.43
ATOM	1777	CG	PRO	A	235	40.982	45.221	44.950	1.00	49.98
ATOM	1778	C	PRO	A	235	39.158	46.887	42.183	1.00	49.94
ATOM	1779	O	PRO	A	235	38.131	46.656	41.550	1.00	52.13
ATOM	1780	N	LEU	A	236	39.685	48.101	42.260	1.00	48.41
ATOM	1781	CA	LEU	A	236	39.062	49.215	41.567	1.00	47.60
ATOM	1782	CB	LEU	A	236	39.801	50.520	41.874	1.00	47.97
ATOM	1783	CG	LEU	A	236	39.349	51.706	41.022	1.00	47.55
ATOM	1784	CD1	LEU	A	236	37.896	52.055	41.340	1.00	47.17
ATOM	1785	CD2	LEU	A	236	40.253	52.888	41.287	1.00	47.75
ATOM	1786	C	LEU	A	236	39.073	48.964	40.055	1.00	45.72
ATOM	1787	O	LEU	A	236	38.076	49.184	39.376	1.00	44.72
ATOM	1788	N	TYR	A	237	40.198	48.501	39.530	1.00	44.51

133/396

Figure 2A-33

ATOM	1789	CA	TYR	A	237	40.299	48.244	38.098	1.00	46.21
ATOM	1790	CB	TYR	A	237	41.719	47.837	37.735	1.00	46.00
ATOM	1791	CG	TYR	A	237	41.891	47.554	36.262	1.00	43.46
ATOM	1792	CD1	TYR	A	237	41.693	48.558	35.318	1.00	41.05
ATOM	1793	CE1	TYR	A	237	41.811	48.300	33.959	1.00	39.34
ATOM	1794	CD2	TYR	A	237	42.213	46.279	35.811	1.00	39.29
ATOM	1795	CE2	TYR	A	237	42.330	46.008	34.455	1.00	42.77
ATOM	1796	CZ	TYR	A	237	42.129	47.026	33.530	1.00	42.84
ATOM	1797	OH	TYR	A	237	42.275	46.777	32.180	1.00	39.98
ATOM	1798	C	TYR	A	237	39.329	47.168	37.614	1.00	48.83
ATOM	1799	O	TYR	A	237	38.615	47.378	36.633	1.00	50.09
ATOM	1800	N	GLU	A	238	39.312	46.021	38.296	1.00	49.13
ATOM	1801	CA	GLU	A	238	38.414	44.913	37.958	1.00	50.04
ATOM	1802	CB	GLU	A	238	38.478	43.809	39.020	1.00	48.22
ATOM	1803	CG	GLU	A	238	39.780	43.078	39.100	1.00	57.55
ATOM	1804	CD	GLU	A	238	39.735	41.917	40.091	1.00	63.55
ATOM	1805	OE1	GLU	A	238	40.778	41.232	40.250	1.00	66.03
ATOM	1806	OE2	GLU	A	238	38.665	41.694	40.706	1.00	62.18
ATOM	1807	C	GLU	A	238	36.963	45.375	37.855	1.00	49.76
ATOM	1808	O	GLU	A	238	36.235	44.935	36.967	1.00	51.72
ATOM	1809	N	HIS	A	239	36.544	46.233	38.783	1.00	46.51
ATOM	1810	CA	HIS	A	239	35.185	46.752	38.796	1.00	47.26
ATOM	1811	CB	HIS	A	239	34.882	47.412	40.139	1.00	49.06
ATOM	1812	CG	HIS	A	239	34.466	46.439	41.195	1.00	51.38
ATOM	1813	CD2	HIS	A	239	35.151	45.892	42.223	1.00	49.97
ATOM	1814	ND1	HIS	A	239	33.219	45.854	41.211	1.00	52.99
ATOM	1815	CE1	HIS	A	239	33.154	44.985	42.204	1.00	50.76
ATOM	1816	NE2	HIS	A	239	34.315	44.989	42.833	1.00	53.82
ATOM	1817	C	HIS	A	239	34.951	47.750	37.674	1.00	48.47
ATOM	1818	O	HIS	A	239	33.833	47.889	37.161	1.00	49.84
ATOM	1819	N	LEU	A	240	36.010	48.448	37.299	1.00	44.79
ATOM	1820	CA	LEU	A	240	35.920	49.408	36.227	1.00	43.92
ATOM	1821	CB	LEU	A	240	37.171	50.295	36.235	1.00	44.27
ATOM	1822	CG	LEU	A	240	37.218	51.534	35.337	1.00	43.81
ATOM	1823	CD1	LEU	A	240	37.885	51.207	34.057	1.00	46.61
ATOM	1824	CD2	LEU	A	240	35.829	52.076	35.120	1.00	42.34
ATOM	1825	C	LEU	A	240	35.851	48.554	34.966	1.00	40.20
ATOM	1826	O	LEU	A	240	35.101	48.833	34.046	1.00	39.69
ATOM	1827	N	HIS	A	241	36.636	47.489	34.965	1.00	39.48
ATOM	1828	CA	HIS	A	241	36.711	46.561	33.853	1.00	40.70
ATOM	1829	CB	HIS	A	241	37.820	45.552	34.146	1.00	40.48
ATOM	1830	CG	HIS	A	241	37.983	44.501	33.097	1.00	42.23
ATOM	1831	CD2	HIS	A	241	38.988	44.265	32.224	1.00	44.20
ATOM	1832	ND1	HIS	A	241	37.046	43.513	32.881	1.00	42.86
ATOM	1833	CE1	HIS	A	241	37.469	42.713	31.920	1.00	42.38
ATOM	1834	NE2	HIS	A	241	38.646	43.146	31.505	1.00	45.88
ATOM	1835	C	HIS	A	241	35.376	45.852	33.603	1.00	43.09
ATOM	1836	O	HIS	A	241	34.933	45.748	32.459	1.00	43.73
ATOM	1837	N	ALA	A	242	34.745	45.378	34.679	1.00	44.26
ATOM	1838	CA	ALA	A	242	33.465	44.678	34.609	1.00	45.42
ATOM	1839	CB	ALA	A	242	33.103	44.105	35.975	1.00	44.29
ATOM	1840	C	ALA	A	242	32.367	45.611	34.143	1.00	45.67
ATOM	1841	O	ALA	A	242	31.465	45.215	33.415	1.00	50.04
ATOM	1842	N	TYR	A	243	32.440	46.860	34.566	1.00	46.54
ATOM	1843	CA	TYR	A	243	31.435	47.819	34.167	1.00	45.03
ATOM	1844	CB	TYR	A	243	31.502	49.060	35.063	1.00	40.49

134/396

Figure 2A-34

ATOM	1845	CG	TYR	A	243	30.655	50.217	34.584	1.00	36.56
ATOM	1846	CD1	TYR	A	243	29.286	50.261	34.838	1.00	37.57
ATOM	1847	CE1	TYR	A	243	28.491	51.327	34.372	1.00	43.87
ATOM	1848	CD2	TYR	A	243	31.223	51.259	33.855	1.00	35.21
ATOM	1849	CE2	TYR	A	243	30.448	52.322	33.386	1.00	44.41
ATOM	1850	CZ	TYR	A	243	29.084	52.348	33.647	1.00	44.83
ATOM	1851	OH	TYR	A	243	28.321	53.390	33.173	1.00	49.51
ATOM	1852	C	TYR	A	243	31.586	48.216	32.694	1.00	47.45
ATOM	1853	O	TYR	A	243	30.594	48.260	31.961	1.00	47.75
ATOM	1854	N	VAL	A	244	32.801	48.500	32.236	1.00	46.27
ATOM	1855	CA	VAL	A	244	32.903	48.893	30.842	1.00	47.13
ATOM	1856	CB	VAL	A	244	34.261	49.586	30.486	1.00	47.01
ATOM	1857	CG1	VAL	A	244	34.728	50.518	31.642	1.00	40.48
ATOM	1858	CG2	VAL	A	244	35.294	48.558	30.115	1.00	48.31
ATOM	1859	C	VAL	A	244	32.681	47.658	29.972	1.00	47.57
ATOM	1860	O	VAL	A	244	32.068	47.749	28.920	1.00	44.97
ATOM	1861	N	ARG	A	245	33.157	46.500	30.418	1.00	49.18
ATOM	1862	CA	ARG	A	245	32.952	45.276	29.647	1.00	52.96
ATOM	1863	CB	ARG	A	245	33.609	44.076	30.349	1.00	51.15
ATOM	1864	CG	ARG	A	245	32.657	43.062	30.915	1.00	56.01
ATOM	1865	CD	ARG	A	245	32.832	41.698	30.285	1.00	47.34
ATOM	1866	NE	ARG	A	245	34.000	40.979	30.774	1.00	48.41
ATOM	1867	CZ	ARG	A	245	34.220	40.657	32.047	1.00	43.87
ATOM	1868	NH1	ARG	A	245	35.319	39.994	32.389	1.00	43.32
ATOM	1869	NH2	ARG	A	245	33.355	41.001	32.978	1.00	42.55
ATOM	1870	C	ARG	A	245	31.450	45.022	29.410	1.00	54.98
ATOM	1871	O	ARG	A	245	31.061	44.520	28.354	1.00	55.80
ATOM	1872	N	ALA	A	246	30.605	45.371	30.381	1.00	54.53
ATOM	1873	CA	ALA	A	246	29.164	45.183	30.213	1.00	54.63
ATOM	1874	CB	ALA	A	246	28.456	45.274	31.555	1.00	55.02
ATOM	1875	C	ALA	A	246	28.590	46.223	29.243	1.00	55.19
ATOM	1876	O	ALA	A	246	27.647	45.941	28.497	1.00	53.30
ATOM	1877	N	LYS	A	247	29.163	47.424	29.258	1.00	53.53
ATOM	1878	CA	LYS	A	247	28.722	48.493	28.378	1.00	54.01
ATOM	1879	CB	LYS	A	247	29.325	49.829	28.813	1.00	55.52
ATOM	1880	CG	LYS	A	247	28.691	50.418	30.059	1.00	60.54
ATOM	1881	CD	LYS	A	247	27.272	50.888	29.784	1.00	63.36
ATOM	1882	CE	LYS	A	247	26.665	51.555	31.008	1.00	64.88
ATOM	1883	NZ	LYS	A	247	25.280	52.047	30.732	1.00	67.29
ATOM	1884	C	LYS	A	247	29.127	48.196	26.943	1.00	53.24
ATOM	1885	O	LYS	A	247	28.358	48.450	26.013	1.00	54.10
ATOM	1886	N	LEU	A	248	30.332	47.660	26.764	1.00	50.30
ATOM	1887	CA	LEU	A	248	30.827	47.327	25.432	1.00	50.96
ATOM	1888	CB	LEU	A	248	32.320	46.986	25.472	1.00	46.03
ATOM	1889	CG	LEU	A	248	33.330	48.131	25.643	1.00	49.58
ATOM	1890	CD1	LEU	A	248	34.742	47.558	25.761	1.00	43.10
ATOM	1891	CD2	LEU	A	248	33.239	49.087	24.456	1.00	49.15
ATOM	1892	C	LEU	A	248	30.045	46.158	24.826	1.00	53.65
ATOM	1893	O	LEU	A	248	30.052	45.965	23.605	1.00	54.57
ATOM	1894	N	MET	A	249	29.383	45.372	25.671	1.00	54.54
ATOM	1895	CA	MET	A	249	28.593	44.257	25.168	1.00	57.94
ATOM	1896	CB	MET	A	249	28.191	43.307	26.296	1.00	56.23
ATOM	1897	CG	MET	A	249	29.350	42.456	26.776	1.00	59.25
ATOM	1898	SD	MET	A	249	28.897	41.264	28.046	1.00	62.91
ATOM	1899	CE	MET	A	249	28.527	42.325	29.411	1.00	63.28
ATOM	1900	C	MET	A	249	27.359	44.796	24.457	1.00	57.52

135/396

Figure 2A-35

ATOM	1901	O	MET	A	249	26.919	44.230	23.461	1.00	59.40
ATOM	1902	N	ASN	A	250	26.813	45.901	24.950	1.00	57.79
ATOM	1903	CA	ASN	A	250	25.647	46.490	24.307	1.00	58.14
ATOM	1904	CB	ASN	A	250	25.001	47.571	25.192	1.00	58.23
ATOM	1905	CG	ASN	A	250	24.484	47.020	26.525	1.00	62.17
ATOM	1906	OD1	ASN	A	250	24.155	45.834	26.646	1.00	59.01
ATOM	1907	ND2	ASN	A	250	24.391	47.894	27.526	1.00	61.67
ATOM	1908	C	ASN	A	250	26.086	47.105	22.981	1.00	58.41
ATOM	1909	O	ASN	A	250	25.379	47.006	21.974	1.00	56.38
ATOM	1910	N	ALA	A	251	27.267	47.724	22.984	1.00	57.70
ATOM	1911	CA	ALA	A	251	27.815	48.369	21.787	1.00	55.51
ATOM	1912	CB	ALA	A	251	28.996	49.262	22.164	1.00	54.22
ATOM	1913	C	ALA	A	251	28.247	47.381	20.705	1.00	54.29
ATOM	1914	O	ALA	A	251	28.197	47.701	19.521	1.00	56.18
ATOM	1915	N	TYR	A	252	28.670	46.189	21.113	1.00	52.78
ATOM	1916	CA	TYR	A	252	29.128	45.158	20.183	1.00	51.69
ATOM	1917	CB	TYR	A	252	30.645	44.999	20.315	1.00	50.06
ATOM	1918	CG	TYR	A	252	31.419	46.247	19.939	1.00	48.71
ATOM	1919	CD1	TYR	A	252	31.535	46.647	18.611	1.00	41.90
ATOM	1920	CE1	TYR	A	252	32.230	47.807	18.266	1.00	44.19
ATOM	1921	CD2	TYR	A	252	32.019	47.045	20.923	1.00	50.73
ATOM	1922	CE2	TYR	A	252	32.718	48.211	20.587	1.00	44.96
ATOM	1923	CZ	TYR	A	252	32.822	48.585	19.260	1.00	47.44
ATOM	1924	OH	TYR	A	252	33.541	49.726	18.926	1.00	47.12
ATOM	1925	C	TYR	A	252	28.420	43.831	20.484	1.00	52.28
ATOM	1926	O	TYR	A	252	29.046	42.831	20.849	1.00	50.55
ATOM	1927	N	PRO	A	253	27.093	43.808	20.316	1.00	54.17
ATOM	1928	CD	PRO	A	253	26.296	44.882	19.697	1.00	54.11
ATOM	1929	CA	PRO	A	253	26.266	42.624	20.572	1.00	54.94
ATOM	1930	CB	PRO	A	253	24.940	42.986	19.916	1.00	55.09
ATOM	1931	CG	PRO	A	253	24.888	44.471	20.043	1.00	54.52
ATOM	1932	C	PRO	A	253	26.839	41.317	20.030	1.00	55.82
ATOM	1933	O	PRO	A	253	27.146	41.218	18.850	1.00	54.25
ATOM	1934	N	SER	A	254	26.977	40.330	20.913	1.00	57.14
ATOM	1935	CA	SER	A	254	27.478	39.001	20.573	1.00	59.74
ATOM	1936	CB	SER	A	254	26.621	38.401	19.454	1.00	63.51
ATOM	1937	OG	SER	A	254	25.328	38.072	19.950	1.00	67.83
ATOM	1938	C	SER	A	254	28.952	38.862	20.214	1.00	59.06
ATOM	1939	O	SER	A	254	29.379	37.836	19.691	1.00	61.52
ATOM	1940	N	TYR	A	255	29.738	39.883	20.504	1.00	58.68
ATOM	1941	CA	TYR	A	255	31.162	39.828	20.210	1.00	57.44
ATOM	1942	CB	TYR	A	255	31.619	41.135	19.537	1.00	57.13
ATOM	1943	CG	TYR	A	255	31.340	41.223	18.045	1.00	58.08
ATOM	1944	CD1	TYR	A	255	30.561	42.255	17.517	1.00	59.07
ATOM	1945	CE1	TYR	A	255	30.363	42.377	16.131	1.00	56.45
ATOM	1946	CD2	TYR	A	255	31.911	40.308	17.153	1.00	58.65
ATOM	1947	CE2	TYR	A	255	31.722	40.421	15.782	1.00	55.66
ATOM	1948	CZ	TYR	A	255	30.949	41.457	15.275	1.00	59.19
ATOM	1949	OH	TYR	A	255	30.784	41.577	13.907	1.00	58.20
ATOM	1950	C	TYR	A	255	31.995	39.603	21.466	1.00	55.40
ATOM	1951	O	TYR	A	255	33.124	39.134	21.378	1.00	57.29
ATOM	1952	N	ILE	A	256	31.432	39.911	22.633	1.00	54.36
ATOM	1953	CA	ILE	A	256	32.181	39.802	23.886	1.00	53.60
ATOM	1954	CB	ILE	A	256	32.392	41.211	24.487	1.00	51.19
ATOM	1955	CG2	ILE	A	256	33.194	41.118	25.786	1.00	50.94
ATOM	1956	CG1	ILE	A	256	33.108	42.097	23.470	1.00	50.60

136/396

Figure 2A-36

ATOM	1957	CD1	ILE	A	256	33.032	43.574	23.800	1.00	51.97
ATOM	1958	C	ILE	A	256	31.552	38.913	24.962	1.00	52.27
ATOM	1959	O	ILE	A	256	30.360	38.987	25.212	1.00	54.15
ATOM	1960	N	SER	A	257	32.376	38.095	25.606	1.00	51.59
ATOM	1961	CA	SER	A	257	31.927	37.196	26.665	1.00	52.29
ATOM	1962	CB	SER	A	257	32.936	36.063	26.822	1.00	49.18
ATOM	1963	OG	SER	A	257	32.695	35.312	28.000	1.00	55.29
ATOM	1964	C	SER	A	257	31.751	37.935	28.010	1.00	54.14
ATOM	1965	O	SER	A	257	32.523	38.831	28.352	1.00	54.78
ATOM	1966	N	PRO	A	258	30.719	37.570	28.781	1.00	54.64
ATOM	1967	CD	PRO	A	258	29.664	36.613	28.403	1.00	56.70
ATOM	1968	CA	PRO	A	258	30.425	38.181	30.085	1.00	53.10
ATOM	1969	CB	PRO	A	258	29.110	37.503	30.501	1.00	57.33
ATOM	1970	CG	PRO	A	258	28.479	37.122	29.179	1.00	57.69
ATOM	1971	C	PRO	A	258	31.521	37.927	31.105	1.00	49.61
ATOM	1972	O	PRO	A	258	31.596	38.601	32.138	1.00	48.03
ATOM	1973	N	ILE	A	259	32.356	36.934	30.832	1.00	47.06
ATOM	1974	CA	ILE	A	259	33.425	36.611	31.758	1.00	48.68
ATOM	1975	CB	ILE	A	259	33.312	35.160	32.257	1.00	48.83
ATOM	1976	CG2	ILE	A	259	31.939	34.930	32.883	1.00	46.34
ATOM	1977	CG1	ILE	A	259	33.582	34.197	31.094	1.00	49.95
ATOM	1978	CD1	ILE	A	259	34.023	32.806	31.535	1.00	50.49
ATOM	1979	C	ILE	A	259	34.812	36.767	31.146	1.00	48.19
ATOM	1980	O	ILE	A	259	35.820	36.546	31.827	1.00	48.03
ATOM	1981	N	GLY	A	260	34.867	37.152	29.875	1.00	46.56
ATOM	1982	CA	GLY	A	260	36.153	37.265	29.217	1.00	48.38
ATOM	1983	C	GLY	A	260	36.842	38.616	29.190	1.00	50.85
ATOM	1984	O	GLY	A	260	36.278	39.648	29.574	1.00	51.22
ATOM	1985	N	CYS	A	261	38.095	38.586	28.747	1.00	49.61
ATOM	1986	CA	CYS	A	261	38.897	39.786	28.600	1.00	48.76
ATOM	1987	CB	CYS	A	261	40.315	39.423	28.166	1.00	44.94
ATOM	1988	SG	CYS	A	261	41.321	38.567	29.419	1.00	54.84
ATOM	1989	C	CYS	A	261	38.260	40.648	27.506	1.00	49.66
ATOM	1990	O	CYS	A	261	37.462	40.165	26.694	1.00	48.02
ATOM	1991	N	LEU	A	262	38.623	41.923	27.493	1.00	46.36
ATOM	1992	CA	LEU	A	262	38.125	42.849	26.501	1.00	47.30
ATOM	1993	CB	LEU	A	262	38.259	44.282	27.009	1.00	47.53
ATOM	1994	CG	LEU	A	262	37.458	44.552	28.278	1.00	50.71
ATOM	1995	CD1	LEU	A	262	37.774	45.953	28.830	1.00	44.60
ATOM	1996	CD2	LEU	A	262	35.966	44.383	27.949	1.00	47.73
ATOM	1997	C	LEU	A	262	38.968	42.680	25.254	1.00	45.63
ATOM	1998	O	LEU	A	262	40.183	42.594	25.341	1.00	45.37
ATOM	1999	N	PRO	A	263	38.330	42.583	24.080	1.00	46.26
ATOM	2000	CD	PRO	A	263	36.903	42.317	23.822	1.00	46.84
ATOM	2001	CA	PRO	A	263	39.119	42.431	22.856	1.00	47.45
ATOM	2002	CB	PRO	A	263	38.047	42.286	21.779	1.00	49.64
ATOM	2003	CG	PRO	A	263	36.959	41.535	22.516	1.00	48.33
ATOM	2004	C	PRO	A	263	39.986	43.689	22.687	1.00	46.31
ATOM	2005	O	PRO	A	263	39.500	44.810	22.823	1.00	46.18
ATOM	2006	N	ALA	A	264	41.268	43.489	22.398	1.00	45.08
ATOM	2007	CA	ALA	A	264	42.227	44.582	22.251	1.00	43.62
ATOM	2008	CB	ALA	A	264	43.572	43.995	21.885	1.00	43.70
ATOM	2009	C	ALA	A	264	41.887	45.745	21.291	1.00	44.21
ATOM	2010	O	ALA	A	264	42.296	46.899	21.535	1.00	42.16
ATOM	2011	N	HIS	A	265	41.140	45.460	20.223	1.00	41.05
ATOM	2012	CA	HIS	A	265	40.796	46.487	19.231	1.00	39.35

137/396

Figure 2A-37

ATOM	2013	CB	HIS	A	265	40.642	45.838	17.847	1.00	44.20
ATOM	2014	CG	HIS	A	265	39.459	44.924	17.736	1.00	44.25
ATOM	2015	CD2	HIS	A	265	38.389	44.945	16.903	1.00	48.08
ATOM	2016	ND1	HIS	A	265	39.294	43.818	18.541	1.00	44.82
ATOM	2017	CE1	HIS	A	265	38.177	43.194	18.209	1.00	49.78
ATOM	2018	NE2	HIS	A	265	37.608	43.858	17.216	1.00	49.17
ATOM	2019	C	HIS	A	265	39.553	47.313	19.518	1.00	39.35
ATOM	2020	O	HIS	A	265	39.172	48.138	18.700	1.00	37.90
ATOM	2021	N	LEU	A	266	38.923	47.107	20.672	1.00	41.44
ATOM	2022	CA	LEU	A	266	37.707	47.841	21.008	1.00	42.55
ATOM	2023	CB	LEU	A	266	36.598	46.843	21.389	1.00	43.54
ATOM	2024	CG	LEU	A	266	36.286	45.689	20.413	1.00	44.72
ATOM	2025	CD1	LEU	A	266	35.149	44.811	20.954	1.00	41.72
ATOM	2026	CD2	LEU	A	266	35.899	46.252	19.066	1.00	42.96
ATOM	2027	C	LEU	A	266	37.855	48.854	22.152	1.00	44.09
ATOM	2028	O	LEU	A	266	36.854	49.280	22.718	1.00	44.54
ATOM	2029	N	LEU	A	267	39.077	49.272	22.475	1.00	46.92
ATOM	2030	CA	LEU	A	267	39.280	50.161	23.629	1.00	45.13
ATOM	2031	CB	LEU	A	267	40.467	49.658	24.437	1.00	42.64
ATOM	2032	CG	LEU	A	267	40.440	48.173	24.801	1.00	44.58
ATOM	2033	CD1	LEU	A	267	41.843	47.754	25.266	1.00	41.41
ATOM	2034	CD2	LEU	A	267	39.381	47.907	25.862	1.00	40.31
ATOM	2035	C	LEU	A	267	39.424	51.675	23.464	1.00	46.48
ATOM	2036	O	LEU	A	267	39.684	52.374	24.446	1.00	45.89
ATOM	2037	N	GLY	A	268	39.299	52.211	22.262	1.00	44.02
ATOM	2038	CA	GLY	A	268	39.392	53.658	22.192	1.00	46.87
ATOM	2039	C	GLY	A	268	40.636	54.265	21.597	1.00	43.11
ATOM	2040	O	GLY	A	268	40.652	55.451	21.300	1.00	46.47
ATOM	2041	N	ASP	A	269	41.699	53.489	21.484	1.00	41.14
ATOM	2042	CA	ASP	A	269	42.887	53.983	20.824	1.00	41.22
ATOM	2043	CB	ASP	A	269	43.777	54.901	21.723	1.00	43.83
ATOM	2044	CG	ASP	A	269	44.596	54.168	22.802	1.00	46.20
ATOM	2045	OD1	ASP	A	269	44.849	54.839	23.826	1.00	47.52
ATOM	2046	OD2	ASP	A	269	45.034	53.006	22.650	1.00	41.15
ATOM	2047	C	ASP	A	269	43.559	52.754	20.274	1.00	37.64
ATOM	2048	O	ASP	A	269	43.066	51.647	20.473	1.00	40.14
ATOM	2049	N	MET	A	270	44.652	52.928	19.564	1.00	36.26
ATOM	2050	CA	MET	A	270	45.284	51.797	18.923	1.00	39.18
ATOM	2051	CB	MET	A	270	46.386	52.319	18.004	1.00	35.65
ATOM	2052	CG	MET	A	270	47.110	51.241	17.165	1.00	40.80
ATOM	2053	SD	MET	A	270	45.981	50.329	16.077	1.00	41.96
ATOM	2054	CE	MET	A	270	46.206	51.283	14.585	1.00	43.33
ATOM	2055	C	MET	A	270	45.822	50.676	19.818	1.00	41.85
ATOM	2056	O	MET	A	270	46.090	49.571	19.328	1.00	41.79
ATOM	2057	N	TRP	A	271	45.930	50.929	21.120	1.00	40.15
ATOM	2058	CA	TRP	A	271	46.532	49.941	22.017	1.00	41.34
ATOM	2059	CB	TRP	A	271	47.932	50.417	22.433	1.00	38.04
ATOM	2060	CG	TRP	A	271	48.795	50.912	21.308	1.00	38.97
ATOM	2061	CD2	TRP	A	271	48.847	52.247	20.788	1.00	34.80
ATOM	2062	CE2	TRP	A	271	49.759	52.243	19.717	1.00	37.07
ATOM	2063	CE3	TRP	A	271	48.210	53.448	21.132	1.00	38.93
ATOM	2064	CD1	TRP	A	271	49.662	50.173	20.547	1.00	38.16
ATOM	2065	NE1	TRP	A	271	50.242	50.966	19.588	1.00	38.63
ATOM	2066	CZ2	TRP	A	271	50.053	53.394	18.979	1.00	38.71
ATOM	2067	CZ3	TRP	A	271	48.505	54.598	20.399	1.00	33.79
ATOM	2068	CH2	TRP	A	271	49.415	54.559	19.338	1.00	35.84

138/396

Figure 2A-38

ATOM	2069	C	TRP	A	271	45.742	49.695	23.290	1.00	43.27
ATOM	2070	O	TRP	A	271	45.932	48.675	23.960	1.00	44.81
ATOM	2071	N	GLY	A	272	44.851	50.621	23.619	1.00	41.47
ATOM	2072	CA	GLY	A	272	44.125	50.507	24.864	1.00	40.06
ATOM	2073	C	GLY	A	272	44.960	51.180	25.965	1.00	40.89
ATOM	2074	O	GLY	A	272	44.847	50.836	27.150	1.00	41.26
ATOM	2075	N	ARG	A	273	45.810	52.133	25.576	1.00	37.91
ATOM	2076	CA	ARG	A	273	46.639	52.850	26.532	1.00	40.09
ATOM	2077	CB	ARG	A	273	47.597	53.810	25.826	1.00	40.91
ATOM	2078	CG	ARG	A	273	48.584	54.433	26.786	1.00	39.58
ATOM	2079	CD	ARG	A	273	49.475	55.470	26.142	1.00	44.75
ATOM	2080	NE	ARG	A	273	50.299	56.110	27.160	1.00	40.82
ATOM	2081	CZ	ARG	A	273	50.942	57.254	26.999	1.00	41.99
ATOM	2082	NH1	ARG	A	273	51.669	57.738	27.998	1.00	43.38
ATOM	2083	NH2	ARG	A	273	50.857	57.917	25.850	1.00	41.62
ATOM	2084	C	ARG	A	273	45.746	53.630	27.476	1.00	41.47
ATOM	2085	O	ARG	A	273	45.990	53.675	28.697	1.00	37.65
ATOM	2086	N	PHE	A	274	44.712	54.249	26.908	1.00	38.82
ATOM	2087	CA	PHE	A	274	43.737	55.004	27.698	1.00	38.62
ATOM	2088	CB	PHE	A	274	43.882	56.506	27.455	1.00	37.35
ATOM	2089	CG	PHE	A	274	45.252	57.045	27.737	1.00	38.78
ATOM	2090	CD1	PHE	A	274	46.033	57.542	26.704	1.00	37.07
ATOM	2091	CD2	PHE	A	274	45.737	57.119	29.054	1.00	38.00
ATOM	2092	CE1	PHE	A	274	47.285	58.122	26.962	1.00	40.08
ATOM	2093	CE2	PHE	A	274	46.985	57.690	29.333	1.00	34.36
ATOM	2094	CZ	PHE	A	274	47.762	58.197	28.288	1.00	40.86
ATOM	2095	C	PHE	A	274	42.365	54.554	27.204	1.00	37.41
ATOM	2096	O	PHE	A	274	42.249	54.163	26.056	1.00	38.47
ATOM	2097	N	TRP	A	275	41.347	54.587	28.065	1.00	36.78
ATOM	2098	CA	TRP	A	275	39.993	54.193	27.674	1.00	37.41
ATOM	2099	CB	TRP	A	275	39.353	53.263	28.718	1.00	35.85
ATOM	2100	CG	TRP	A	275	39.964	51.906	28.795	1.00	38.76
ATOM	2101	CD2	TRP	A	275	39.645	50.872	29.741	1.00	40.70
ATOM	2102	CE2	TRP	A	275	40.468	49.761	29.440	1.00	39.92
ATOM	2103	CE3	TRP	A	275	38.744	50.775	30.808	1.00	41.22
ATOM	2104	CD1	TRP	A	275	40.938	51.392	27.981	1.00	36.87
ATOM	2105	NE1	TRP	A	275	41.246	50.106	28.364	1.00	37.97
ATOM	2106	CZ2	TRP	A	275	40.415	48.563	30.172	1.00	39.90
ATOM	2107	CZ3	TRP	A	275	38.690	49.577	31.537	1.00	44.51
ATOM	2108	CH2	TRP	A	275	39.522	48.490	31.210	1.00	41.48
ATOM	2109	C	TRP	A	275	39.138	55.446	27.511	1.00	38.04
ATOM	2110	O	TRP	A	275	37.908	55.378	27.398	1.00	36.92
ATOM	2111	N	THR	A	276	39.812	56.591	27.496	1.00	39.31
ATOM	2112	CA	THR	A	276	39.168	57.893	27.335	1.00	43.17
ATOM	2113	CB	THR	A	276	40.185	58.955	26.856	1.00	44.10
ATOM	2114	OG1	THR	A	276	41.398	58.842	27.608	1.00	46.24
ATOM	2115	CG2	THR	A	276	39.613	60.347	27.026	1.00	39.13
ATOM	2116	C	THR	A	276	38.028	57.903	26.310	1.00	42.17
ATOM	2117	O	THR	A	276	36.925	58.356	26.591	1.00	42.27
ATOM	2118	N	ASN	A	277	38.309	57.416	25.111	1.00	43.76
ATOM	2119	CA	ASN	A	277	37.306	57.426	24.046	1.00	46.62
ATOM	2120	CB	ASN	A	277	38.000	57.226	22.702	1.00	44.28
ATOM	2121	CG	ASN	A	277	39.060	58.285	22.446	1.00	44.45
ATOM	2122	OD1	ASN	A	277	40.143	58.002	21.909	1.00	42.75
ATOM	2123	ND2	ASN	A	277	38.755	59.512	22.832	1.00	41.85
ATOM	2124	C	ASN	A	277	36.143	56.453	24.200	1.00	47.07

139/396

Figure 2A-39

ATOM	2125	O	ASN	A	277	35.286	56.377	23.333	1.00	50.40
ATOM	2126	N	LEU	A	278	36.109	55.723	25.308	1.00	46.63
ATOM	2127	CA	LEU	A	278	35.027	54.788	25.583	1.00	45.57
ATOM	2128	CB	LEU	A	278	35.546	53.612	26.427	1.00	44.99
ATOM	2129	CG	LEU	A	278	35.769	52.239	25.783	1.00	45.87
ATOM	2130	CD1	LEU	A	278	36.203	52.397	24.343	1.00	38.74
ATOM	2131	CD2	LEU	A	278	36.772	51.440	26.586	1.00	40.99
ATOM	2132	C	LEU	A	278	33.954	55.529	26.364	1.00	45.28
ATOM	2133	O	LEU	A	278	32.988	54.927	26.832	1.00	49.33
ATOM	2134	N	TYR	A	279	34.106	56.839	26.500	1.00	43.55
ATOM	2135	CA	TYR	A	279	33.146	57.606	27.283	1.00	46.28
ATOM	2136	CB	TYR	A	279	33.646	59.035	27.497	1.00	41.83
ATOM	2137	CG	TYR	A	279	32.854	59.756	28.550	1.00	42.27
ATOM	2138	CD1	TYR	A	279	32.897	59.346	29.874	1.00	43.29
ATOM	2139	CE1	TYR	A	279	32.147	59.997	30.854	1.00	47.07
ATOM	2140	CD2	TYR	A	279	32.029	60.842	28.219	1.00	48.46
ATOM	2141	CE2	TYR	A	279	31.267	61.501	29.193	1.00	45.25
ATOM	2142	CZ	TYR	A	279	31.335	61.073	30.509	1.00	48.66
ATOM	2143	OH	TYR	A	279	30.606	61.718	31.488	1.00	46.96
ATOM	2144	C	TYR	A	279	31.711	57.636	26.754	1.00	48.22
ATOM	2145	O	TYR	A	279	30.764	57.470	27.521	1.00	52.32
ATOM	2146	N	SER	A	280	31.538	57.853	25.459	1.00	51.15
ATOM	2147	CA	SER	A	280	30.194	57.875	24.876	1.00	54.09
ATOM	2148	CB	SER	A	280	30.270	58.283	23.409	1.00	54.73
ATOM	2149	OG	SER	A	280	30.522	59.674	23.300	1.00	62.60
ATOM	2150	C	SER	A	280	29.478	56.520	24.985	1.00	56.26
ATOM	2151	O	SER	A	280	28.248	56.454	25.008	1.00	59.62
ATOM	2152	N	LEU	A	281	30.250	55.443	25.054	1.00	54.56
ATOM	2153	CA	LEU	A	281	29.686	54.113	25.160	1.00	51.49
ATOM	2154	CB	LEU	A	281	30.598	53.086	24.466	1.00	53.21
ATOM	2155	CG	LEU	A	281	31.203	53.322	23.074	1.00	56.24
ATOM	2156	CD1	LEU	A	281	32.215	54.482	23.102	1.00	58.22
ATOM	2157	CD2	LEU	A	281	31.919	52.047	22.624	1.00	53.45
ATOM	2158	C	LEU	A	281	29.521	53.690	26.622	1.00	51.99
ATOM	2159	O	LEU	A	281	28.822	52.714	26.908	1.00	52.46
ATOM	2160	N	THR	A	282	30.154	54.406	27.554	1.00	49.94
ATOM	2161	CA	THR	A	282	30.075	54.006	28.966	1.00	46.49
ATOM	2162	CB	THR	A	282	31.482	53.583	29.503	1.00	47.26
ATOM	2163	OG1	THR	A	282	32.411	54.666	29.340	1.00	45.14
ATOM	2164	CG2	THR	A	282	32.016	52.373	28.763	1.00	41.64
ATOM	2165	C	THR	A	282	29.504	55.027	29.945	1.00	46.78
ATOM	2166	O	THR	A	282	29.278	54.703	31.106	1.00	48.40
ATOM	2167	N	VAL	A	283	29.279	56.256	29.499	1.00	48.11
ATOM	2168	CA	VAL	A	283	28.758	57.288	30.394	1.00	51.25
ATOM	2169	CB	VAL	A	283	28.415	58.589	29.599	1.00	52.46
ATOM	2170	CG1	VAL	A	283	27.394	58.295	28.502	1.00	50.07
ATOM	2171	CG2	VAL	A	283	27.914	59.665	30.549	1.00	53.33
ATOM	2172	C	VAL	A	283	27.545	56.840	31.233	1.00	53.59
ATOM	2173	O	VAL	A	283	26.501	56.482	30.693	1.00	55.34
ATOM	2174	N	PRO	A	284	27.680	56.861	32.577	1.00	53.71
ATOM	2175	CD	PRO	A	284	28.912	57.263	33.283	1.00	51.76
ATOM	2176	CA	PRO	A	284	26.640	56.468	33.537	1.00	53.29
ATOM	2177	CB	PRO	A	284	27.286	56.778	34.886	1.00	54.98
ATOM	2178	CG	PRO	A	284	28.757	56.586	34.618	1.00	51.98
ATOM	2179	C	PRO	A	284	25.271	57.159	33.378	1.00	55.97
ATOM	2180	O	PRO	A	284	24.226	56.513	33.518	1.00	53.70

140/396

Figure 2A-40

ATOM	2181	N	PHE	A	285	25.276	58.466	33.118	1.00	57.15
ATOM	2182	CA	PHE	A	285	24.037	59.227	32.939	1.00	58.11
ATOM	2183	CB	PHE	A	285	23.689	60.016	34.210	1.00	57.90
ATOM	2184	CG	PHE	A	285	23.688	59.178	35.456	1.00	56.08
ATOM	2185	CD1	PHE	A	285	24.849	59.028	36.206	1.00	53.14
ATOM	2186	CD2	PHE	A	285	22.548	58.463	35.828	1.00	55.96
ATOM	2187	CE1	PHE	A	285	24.887	58.168	37.307	1.00	54.09
ATOM	2188	CE2	PHE	A	285	22.567	57.598	36.925	1.00	53.45
ATOM	2189	CZ	PHE	A	285	23.743	57.447	37.668	1.00	56.27
ATOM	2190	C	PHE	A	285	24.198	60.189	31.772	1.00	60.90
ATOM	2191	O	PHE	A	285	24.526	61.364	31.956	1.00	60.11
ATOM	2192	N	GLY	A	286	23.947	59.684	30.569	1.00	64.10
ATOM	2193	CA	GLY	A	286	24.085	60.489	29.367	1.00	67.35
ATOM	2194	C	GLY	A	286	23.237	61.741	29.235	1.00	69.85
ATOM	2195	O	GLY	A	286	23.509	62.581	28.376	1.00	70.95
ATOM	2196	N	GLN	A	287	22.221	61.881	30.078	1.00	72.79
ATOM	2197	CA	GLN	A	287	21.331	63.042	30.025	1.00	76.49
ATOM	2198	CB	GLN	A	287	19.977	62.695	30.646	1.00	78.33
ATOM	2199	CG	GLN	A	287	19.729	61.191	30.796	1.00	81.75
ATOM	2200	CD	GLN	A	287	20.627	60.545	31.848	1.00	80.17
ATOM	2201	OE1	GLN	A	287	20.610	59.330	32.032	1.00	81.68
ATOM	2202	NE2	GLN	A	287	21.407	61.361	32.542	1.00	80.55
ATOM	2203	C	GLN	A	287	21.915	64.254	30.738	1.00	78.04
ATOM	2204	O	GLN	A	287	21.743	65.389	30.289	1.00	77.69
ATOM	2205	N	LYS	A	288	22.595	64.010	31.856	1.00	80.27
ATOM	2206	CA	LYS	A	288	23.207	65.088	32.625	1.00	81.07
ATOM	2207	CB	LYS	A	288	23.852	64.536	33.901	1.00	78.06
ATOM	2208	CG	LYS	A	288	22.862	64.078	34.966	1.00	77.75
ATOM	2209	CD	LYS	A	288	22.169	65.264	35.629	1.00	78.18
ATOM	2210	CE	LYS	A	288	21.080	64.818	36.600	1.00	77.52
ATOM	2211	NZ	LYS	A	288	21.604	63.965	37.702	1.00	78.08
ATOM	2212	C	LYS	A	288	24.261	65.789	31.781	1.00	82.77
ATOM	2213	O	LYS	A	288	25.077	65.141	31.126	1.00	83.13
ATOM	2214	N	PRO	A	289	24.246	67.129	31.769	1.00	85.03
ATOM	2215	CD	PRO	A	289	23.181	68.008	32.276	1.00	85.45
ATOM	2216	CA	PRO	A	289	25.224	67.896	30.988	1.00	86.69
ATOM	2217	CB	PRO	A	289	24.680	69.326	31.049	1.00	86.17
ATOM	2218	CG	PRO	A	289	23.206	69.129	31.266	1.00	87.01
ATOM	2219	C	PRO	A	289	26.630	67.801	31.585	1.00	86.85
ATOM	2220	O	PRO	A	289	26.809	67.886	32.802	1.00	86.21
ATOM	2221	N	ASN	A	290	27.617	67.621	30.716	1.00	86.70
ATOM	2222	CA	ASN	A	290	29.009	67.535	31.129	1.00	87.62
ATOM	2223	CB	ASN	A	290	29.801	66.751	30.080	1.00	89.69
ATOM	2224	CG	ASN	A	290	31.272	66.617	30.428	1.00	90.75
ATOM	2225	OD1	ASN	A	290	31.644	65.895	31.358	1.00	92.36
ATOM	2226	ND2	ASN	A	290	32.119	67.313	29.678	1.00	91.14
ATOM	2227	C	ASN	A	290	29.532	68.970	31.226	1.00	88.01
ATOM	2228	O	ASN	A	290	29.590	69.679	30.217	1.00	88.50
ATOM	2229	N	ILE	A	291	29.896	69.399	32.434	1.00	86.06
ATOM	2230	CA	ILE	A	291	30.404	70.757	32.648	1.00	84.25
ATOM	2231	CB	ILE	A	291	31.091	70.896	34.029	1.00	83.64
ATOM	2232	CG2	ILE	A	291	31.674	72.293	34.178	1.00	84.09
ATOM	2233	CG1	ILE	A	291	30.081	70.633	35.148	1.00	82.38
ATOM	2234	CD1	ILE	A	291	30.647	70.800	36.542	1.00	82.09
ATOM	2235	C	ILE	A	291	31.402	71.167	31.570	1.00	82.57
ATOM	2236	O	ILE	A	291	32.416	70.504	31.363	1.00	83.37

141/396

Figure 2A-41

ATOM	2237	N	ASP	A	292	31.109	72.267	30.886	1.00	81.11
ATOM	2238	CA	ASP	A	292	31.974	72.758	29.820	1.00	80.29
ATOM	2239	CB	ASP	A	292	31.666	72.023	28.515	1.00	78.99
ATOM	2240	CG	ASP	A	292	32.496	72.528	27.361	1.00	80.54
ATOM	2241	OD1	ASP	A	292	32.450	71.913	26.276	1.00	82.13
ATOM	2242	OD2	ASP	A	292	33.195	73.547	27.540	1.00	78.73
ATOM	2243	C	ASP	A	292	31.794	74.259	29.620	1.00	79.63
ATOM	2244	O	ASP	A	292	30.846	74.697	28.969	1.00	79.79
ATOM	2245	N	VAL	A	293	32.725	75.037	30.164	1.00	77.59
ATOM	2246	CA	VAL	A	293	32.666	76.491	30.079	1.00	76.35
ATOM	2247	CB	VAL	A	293	33.384	77.126	31.294	1.00	78.92
ATOM	2248	CG1	VAL	A	293	33.199	78.633	31.281	1.00	81.40
ATOM	2249	CG2	VAL	A	293	32.840	76.541	32.589	1.00	77.90
ATOM	2250	C	VAL	A	293	33.258	77.091	28.797	1.00	74.04
ATOM	2251	O	VAL	A	293	33.392	78.305	28.688	1.00	69.40
ATOM	2252	N	THR	A	294	33.586	76.252	27.820	1.00	73.66
ATOM	2253	CA	THR	A	294	34.179	76.747	26.583	1.00	76.15
ATOM	2254	CB	THR	A	294	34.647	75.575	25.680	1.00	77.48
ATOM	2255	OG1	THR	A	294	35.380	76.094	24.564	1.00	81.36
ATOM	2256	CG2	THR	A	294	33.461	74.780	25.161	1.00	82.40
ATOM	2257	C	THR	A	294	33.243	77.663	25.792	1.00	77.26
ATOM	2258	O	THR	A	294	33.569	78.099	24.685	1.00	74.60
ATOM	2259	N	ASP	A	295	32.086	77.956	26.379	1.00	79.16
ATOM	2260	CA	ASP	A	295	31.081	78.817	25.759	1.00	79.96
ATOM	2261	CB	ASP	A	295	29.743	78.071	25.668	1.00	82.71
ATOM	2262	CG	ASP	A	295	29.806	76.863	24.723	1.00	86.75
ATOM	2263	OD1	ASP	A	295	29.848	77.080	23.491	1.00	82.46
ATOM	2264	OD2	ASP	A	295	29.829	75.701	25.212	1.00	87.00
ATOM	2265	C	ASP	A	295	30.928	80.089	26.582	1.00	78.90
ATOM	2266	O	ASP	A	295	30.753	81.179	26.036	1.00	77.78
ATOM	2267	N	ALA	A	296	31.014	79.942	27.902	1.00	78.90
ATOM	2268	CA	ALA	A	296	30.901	81.070	28.820	1.00	77.24
ATOM	2269	CB	ALA	A	296	30.738	80.566	30.244	1.00	75.71
ATOM	2270	C	ALA	A	296	32.139	81.958	28.714	1.00	78.23
ATOM	2271	O	ALA	A	296	32.105	83.134	29.088	1.00	78.78
ATOM	2272	N	MET	A	297	33.231	81.381	28.216	1.00	78.38
ATOM	2273	CA	MET	A	297	34.484	82.108	28.032	1.00	78.14
ATOM	2274	CB	MET	A	297	35.632	81.133	27.725	1.00	75.84
ATOM	2275	CG	MET	A	297	36.141	80.325	28.931	1.00	73.42
ATOM	2276	SD	MET	A	297	37.220	78.928	28.469	1.00	71.34
ATOM	2277	CE	MET	A	297	38.638	79.782	27.773	1.00	71.30
ATOM	2278	C	MET	A	297	34.279	83.054	26.854	1.00	79.23
ATOM	2279	O	MET	A	297	34.624	84.238	26.912	1.00	78.31
ATOM	2280	N	VAL	A	298	33.706	82.514	25.786	1.00	80.57
ATOM	2281	CA	VAL	A	298	33.432	83.288	24.585	1.00	82.05
ATOM	2282	CB	VAL	A	298	32.746	82.407	23.521	1.00	81.45
ATOM	2283	CG1	VAL	A	298	32.468	83.216	22.263	1.00	79.04
ATOM	2284	CG2	VAL	A	298	33.629	81.210	23.206	1.00	79.69
ATOM	2285	C	VAL	A	298	32.537	84.489	24.903	1.00	83.43
ATOM	2286	O	VAL	A	298	32.930	85.640	24.693	1.00	81.95
ATOM	2287	N	ASP	A	299	31.343	84.212	25.425	1.00	85.20
ATOM	2288	CA	ASP	A	299	30.379	85.259	25.769	1.00	86.86
ATOM	2289	CB	ASP	A	299	29.159	84.641	26.469	1.00	88.91
ATOM	2290	CG	ASP	A	299	28.081	85.676	26.809	1.00	91.60
ATOM	2291	OD1	ASP	A	299	28.046	86.164	27.967	1.00	89.54
ATOM	2292	OD2	ASP	A	299	27.271	86.007	25.909	1.00	92.57

142/396

Figure 2A-42

ATOM	2293	C	ASP	A	299	30.972	86.376	26.636	1.00	86.92
ATOM	2294	O	ASP	A	299	30.458	87.498	26.654	1.00	86.76
ATOM	2295	N	GLN	A	300	32.047	86.075	27.355	1.00	86.74
ATOM	2296	CA	GLN	A	300	32.676	87.085	28.194	1.00	86.19
ATOM	2297	CB	GLN	A	300	33.101	86.481	29.534	1.00	87.50
ATOM	2298	CG	GLN	A	300	31.948	85.867	30.313	1.00	87.08
ATOM	2299	CD	GLN	A	300	32.287	85.610	31.766	1.00	87.34
ATOM	2300	OE1	GLN	A	300	31.491	85.036	32.502	1.00	88.73
ATOM	2301	NE2	GLN	A	300	33.470	86.041	32.190	1.00	86.96
ATOM	2302	C	GLN	A	300	33.877	87.686	27.469	1.00	85.47
ATOM	2303	O	GLN	A	300	34.665	88.432	28.053	1.00	84.91
ATOM	2304	N	ALA	A	301	33.997	87.360	26.186	1.00	83.85
ATOM	2305	CA	ALA	A	301	35.080	87.866	25.359	1.00	83.18
ATOM	2306	CB	ALA	A	301	34.903	89.362	25.123	1.00	83.02
ATOM	2307	C	ALA	A	301	36.427	87.601	26.000	1.00	83.54
ATOM	2308	O	ALA	A	301	37.162	88.536	26.324	1.00	84.30
ATOM	2309	N	TRP	A	302	36.743	86.323	26.192	1.00	83.51
ATOM	2310	CA	TRP	A	302	38.015	85.923	26.785	1.00	81.43
ATOM	2311	CB	TRP	A	302	37.842	84.676	27.657	1.00	81.18
ATOM	2312	CG	TRP	A	302	37.479	84.973	29.082	1.00	79.68
ATOM	2313	CD2	TRP	A	302	37.967	84.300	30.249	1.00	78.80
ATOM	2314	CE2	TRP	A	302	37.317	84.874	31.364	1.00	78.34
ATOM	2315	CE3	TRP	A	302	38.890	83.267	30.462	1.00	78.56
ATOM	2316	CD1	TRP	A	302	36.584	85.902	29.523	1.00	79.53
ATOM	2317	NE1	TRP	A	302	36.480	85.849	30.892	1.00	79.24
ATOM	2318	CZ2	TRP	A	302	37.560	84.450	32.677	1.00	78.27
ATOM	2319	CZ3	TRP	A	302	39.133	82.845	31.772	1.00	78.67
ATOM	2320	CH2	TRP	A	302	38.467	83.438	32.861	1.00	77.32
ATOM	2321	C	TRP	A	302	39.014	85.629	25.688	1.00	80.36
ATOM	2322	O	TRP	A	302	38.647	85.151	24.617	1.00	80.34
ATOM	2323	N	ASP	A	303	40.279	85.922	25.962	1.00	80.02
ATOM	2324	CA	ASP	A	303	41.346	85.681	25.003	1.00	79.38
ATOM	2325	CB	ASP	A	303	41.771	86.996	24.329	1.00	81.57
ATOM	2326	CG	ASP	A	303	41.983	88.127	25.323	1.00	85.07
ATOM	2327	OD1	ASP	A	303	42.935	88.059	26.133	1.00	86.67
ATOM	2328	OD2	ASP	A	303	41.186	89.091	25.296	1.00	87.78
ATOM	2329	C	ASP	A	303	42.536	85.042	25.703	1.00	76.84
ATOM	2330	O	ASP	A	303	42.540	84.890	26.926	1.00	76.08
ATOM	2331	N	ALA	A	304	43.535	84.671	24.912	1.00	72.87
ATOM	2332	CA	ALA	A	304	44.743	84.049	25.417	1.00	71.36
ATOM	2333	CB	ALA	A	304	45.796	84.027	24.322	1.00	69.67
ATOM	2334	C	ALA	A	304	45.278	84.775	26.647	1.00	71.07
ATOM	2335	O	ALA	A	304	45.523	84.163	27.686	1.00	71.69
ATOM	2336	N	GLN	A	305	45.455	86.083	26.528	1.00	70.85
ATOM	2337	CA	GLN	A	305	45.976	86.883	27.631	1.00	70.57
ATOM	2338	CB	GLN	A	305	45.960	88.364	27.251	1.00	72.30
ATOM	2339	CG	GLN	A	305	46.901	88.719	26.113	1.00	77.93
ATOM	2340	CD	GLN	A	305	48.364	88.635	26.511	1.00	78.98
ATOM	2341	OE1	GLN	A	305	48.786	89.234	27.511	1.00	76.97
ATOM	2342	NE2	GLN	A	305	49.152	87.897	25.726	1.00	77.93
ATOM	2343	C	GLN	A	305	45.209	86.687	28.935	1.00	67.99
ATOM	2344	O	GLN	A	305	45.811	86.534	30.002	1.00	66.36
ATOM	2345	N	ARG	A	306	43.882	86.707	28.844	1.00	65.27
ATOM	2346	CA	ARG	A	306	43.030	86.539	30.014	1.00	63.77
ATOM	2347	CB	ARG	A	306	41.572	86.832	29.646	1.00	64.27
ATOM	2348	CG	ARG	A	306	40.593	86.689	30.802	1.00	64.74

143/396

Figure 2A-43

ATOM	2349	CD	ARG	A	306	40.902	87.667	31.924	1.00	66.17
ATOM	2350	NE	ARG	A	306	39.962	87.529	33.032	1.00	66.85
ATOM	2351	CZ	ARG	A	306	38.641	87.627	32.909	1.00	70.02
ATOM	2352	NH1	ARG	A	306	38.095	87.867	31.719	1.00	68.65
ATOM	2353	NH2	ARG	A	306	37.862	87.482	33.977	1.00	69.86
ATOM	2354	C	ARG	A	306	43.156	85.123	30.580	1.00	61.38
ATOM	2355	O	ARG	A	306	43.097	84.927	31.788	1.00	59.81
ATOM	2356	N	ILE	A	307	43.321	84.144	29.697	1.00	60.08
ATOM	2357	CA	ILE	A	307	43.477	82.756	30.112	1.00	60.87
ATOM	2358	CB	ILE	A	307	43.575	81.837	28.889	1.00	58.86
ATOM	2359	CG2	ILE	A	307	44.156	80.485	29.281	1.00	57.42
ATOM	2360	CG1	ILE	A	307	42.188	81.714	28.252	1.00	58.62
ATOM	2361	CD1	ILE	A	307	42.134	80.833	27.041	1.00	57.01
ATOM	2362	C	ILE	A	307	44.729	82.597	30.983	1.00	62.61
ATOM	2363	O	ILE	A	307	44.648	82.081	32.099	1.00	62.60
ATOM	2364	N	PHE	A	308	45.873	83.064	30.483	1.00	62.97
ATOM	2365	CA	PHE	A	308	47.136	82.973	31.221	1.00	64.50
ATOM	2366	CB	PHE	A	308	48.316	83.212	30.277	1.00	60.82
ATOM	2367	CG	PHE	A	308	48.639	82.030	29.411	1.00	59.21
ATOM	2368	CD1	PHE	A	308	49.555	81.068	29.837	1.00	58.36
ATOM	2369	CD2	PHE	A	308	48.001	81.851	28.186	1.00	55.11
ATOM	2370	CE1	PHE	A	308	49.832	79.939	29.056	1.00	55.18
ATOM	2371	CE2	PHE	A	308	48.266	80.734	27.401	1.00	55.92
ATOM	2372	CZ	PHE	A	308	49.186	79.771	27.837	1.00	57.66
ATOM	2373	C	PHE	A	308	47.208	83.937	32.400	1.00	65.93
ATOM	2374	O	PHE	A	308	47.932	83.698	33.372	1.00	68.82
ATOM	2375	N	LYS	A	309	46.453	85.023	32.320	1.00	66.82
ATOM	2376	CA	LYS	A	309	46.441	85.999	33.395	1.00	67.43
ATOM	2377	CB	LYS	A	309	45.785	87.299	32.926	1.00	69.48
ATOM	2378	CG	LYS	A	309	45.909	88.440	33.920	1.00	69.11
ATOM	2379	CD	LYS	A	309	46.852	89.523	33.411	1.00	67.79
ATOM	2380	CE	LYS	A	309	48.199	88.958	33.015	1.00	66.38
ATOM	2381	NZ	LYS	A	309	49.154	90.032	32.617	1.00	67.39
ATOM	2382	C	LYS	A	309	45.652	85.406	34.553	1.00	68.07
ATOM	2383	O	LYS	A	309	45.951	85.662	35.723	1.00	68.65
ATOM	2384	N	GLU	A	310	44.641	84.609	34.223	1.00	66.25
ATOM	2385	CA	GLU	A	310	43.823	83.971	35.250	1.00	65.68
ATOM	2386	CB	GLU	A	310	42.516	83.459	34.631	1.00	69.48
ATOM	2387	CG	GLU	A	310	41.326	83.445	35.584	1.00	72.23
ATOM	2388	CD	GLU	A	310	40.885	84.837	36.023	1.00	73.99
ATOM	2389	OE1	GLU	A	310	40.574	85.678	35.150	1.00	75.33
ATOM	2390	OE2	GLU	A	310	40.836	85.086	37.246	1.00	74.07
ATOM	2391	C	GLU	A	310	44.633	82.819	35.874	1.00	61.86
ATOM	2392	O	GLU	A	310	44.549	82.567	37.070	1.00	58.58
ATOM	2393	N	ALA	A	311	45.425	82.132	35.055	1.00	60.90
ATOM	2394	CA	ALA	A	311	46.274	81.050	35.543	1.00	60.07
ATOM	2395	CB	ALA	A	311	46.980	80.357	34.379	1.00	55.35
ATOM	2396	C	ALA	A	311	47.304	81.676	36.488	1.00	60.87
ATOM	2397	O	ALA	A	311	47.575	81.147	37.565	1.00	62.07
ATOM	2398	N	GLU	A	312	47.868	82.812	36.084	1.00	60.59
ATOM	2399	CA	GLU	A	312	48.853	83.504	36.907	1.00	59.34
ATOM	2400	CB	GLU	A	312	49.376	84.749	36.183	1.00	59.87
ATOM	2401	CG	GLU	A	312	50.347	85.600	37.007	1.00	60.05
ATOM	2402	CD	GLU	A	312	50.797	86.854	36.262	1.00	63.31
ATOM	2403	OE1	GLU	A	312	49.926	87.676	35.905	1.00	65.00
ATOM	2404	OE2	GLU	A	312	52.013	87.017	36.028	1.00	61.02

144/396

Figure 2A-44

ATOM	2405	C	GLU	A	312	48.238	83.906	38.240	1.00	58.21
ATOM	2406	O	GLU	A	312	48.887	83.810	39.291	1.00	58.97
ATOM	2407	N	LYS	A	313	46.987	84.349	38.201	1.00	55.92
ATOM	2408	CA	LYS	A	313	46.306	84.760	39.417	1.00	56.97
ATOM	2409	CB	LYS	A	313	44.980	85.447	39.078	1.00	58.11
ATOM	2410	CG	LYS	A	313	44.205	85.937	40.298	1.00	62.54
ATOM	2411	CD	LYS	A	313	43.031	86.840	39.911	1.00	65.63
ATOM	2412	CE	LYS	A	313	42.265	87.295	41.154	1.00	68.19
ATOM	2413	NZ	LYS	A	313	41.063	88.130	40.839	1.00	70.58
ATOM	2414	C	LYS	A	313	46.067	83.559	40.340	1.00	57.54
ATOM	2415	O	LYS	A	313	46.030	83.704	41.571	1.00	56.07
ATOM	2416	N	PHE	A	314	45.900	82.376	39.747	1.00	55.38
ATOM	2417	CA	PHE	A	314	45.679	81.166	40.529	1.00	51.79
ATOM	2418	CB	PHE	A	314	45.405	79.978	39.607	1.00	54.54
ATOM	2419	CG	PHE	A	314	45.562	78.637	40.281	1.00	53.50
ATOM	2420	CD1	PHE	A	314	44.591	78.160	41.151	1.00	54.88
ATOM	2421	CD2	PHE	A	314	46.693	77.859	40.046	1.00	51.32
ATOM	2422	CE1	PHE	A	314	44.737	76.923	41.779	1.00	55.26
ATOM	2423	CE2	PHE	A	314	46.853	76.625	40.665	1.00	53.62
ATOM	2424	CZ	PHE	A	314	45.871	76.154	41.534	1.00	55.02
ATOM	2425	C	PHE	A	314	46.883	80.850	41.413	1.00	51.39
ATOM	2426	O	PHE	A	314	46.725	80.520	42.583	1.00	51.04
ATOM	2427	N	PHE	A	315	48.085	80.950	40.852	1.00	51.52
ATOM	2428	CA	PHE	A	315	49.303	80.652	41.609	1.00	53.76
ATOM	2429	CB	PHE	A	315	50.487	80.523	40.656	1.00	51.49
ATOM	2430	CG	PHE	A	315	50.388	79.344	39.728	1.00	50.58
ATOM	2431	CD1	PHE	A	315	50.584	78.051	40.201	1.00	52.34
ATOM	2432	CD2	PHE	A	315	50.071	79.521	38.390	1.00	48.98
ATOM	2433	CE1	PHE	A	315	50.460	76.945	39.348	1.00	49.95
ATOM	2434	CE2	PHE	A	315	49.946	78.431	37.535	1.00	48.06
ATOM	2435	CZ	PHE	A	315	50.140	77.141	38.017	1.00	49.47
ATOM	2436	C	PHE	A	315	49.608	81.670	42.709	1.00	56.25
ATOM	2437	O	PHE	A	315	49.909	81.293	43.853	1.00	57.02
ATOM	2438	N	VAL	A	316	49.521	82.954	42.371	1.00	57.13
ATOM	2439	CA	VAL	A	316	49.763	84.014	43.344	1.00	57.45
ATOM	2440	CB	VAL	A	316	49.563	85.422	42.703	1.00	58.57
ATOM	2441	CG1	VAL	A	316	49.498	86.503	43.776	1.00	55.91
ATOM	2442	CG2	VAL	A	316	50.715	85.716	41.755	1.00	57.73
ATOM	2443	C	VAL	A	316	48.797	83.841	44.516	1.00	57.28
ATOM	2444	O	VAL	A	316	49.130	84.140	45.659	1.00	57.53
ATOM	2445	N	SER	A	317	47.604	83.334	44.232	1.00	58.56
ATOM	2446	CA	SER	A	317	46.606	83.136	45.275	1.00	59.07
ATOM	2447	CB	SER	A	317	45.280	82.666	44.675	1.00	59.43
ATOM	2448	OG	SER	A	317	45.324	81.285	44.378	1.00	62.86
ATOM	2449	C	SER	A	317	47.066	82.136	46.332	1.00	60.46
ATOM	2450	O	SER	A	317	46.528	82.124	47.437	1.00	60.30
ATOM	2451	N	VAL	A	318	48.043	81.288	46.005	1.00	59.13
ATOM	2452	CA	VAL	A	318	48.542	80.337	47.004	1.00	59.20
ATOM	2453	CB	VAL	A	318	48.481	78.859	46.513	1.00	57.46
ATOM	2454	CG1	VAL	A	318	47.042	78.456	46.256	1.00	56.84
ATOM	2455	CG2	VAL	A	318	49.328	78.675	45.272	1.00	54.88
ATOM	2456	C	VAL	A	318	49.976	80.649	47.454	1.00	60.35
ATOM	2457	O	VAL	A	318	50.658	79.792	48.033	1.00	57.92
ATOM	2458	N	GLY	A	319	50.432	81.870	47.176	1.00	60.19
ATOM	2459	CA	GLY	A	319	51.763	82.271	47.605	1.00	64.25
ATOM	2460	C	GLY	A	319	52.918	82.192	46.616	1.00	66.40

145/396

Figure 2A-45

ATOM	2461	O	GLY	A	319	54.054	82.552	46.965	1.00	66.55
ATOM	2462	N	LEU	A	320	52.659	81.717	45.401	1.00	65.02
ATOM	2463	CA	LEU	A	320	53.715	81.631	44.401	1.00	63.72
ATOM	2464	CB	LEU	A	320	53.405	80.521	43.385	1.00	61.24
ATOM	2465	CG	LEU	A	320	53.358	79.099	43.964	1.00	61.80
ATOM	2466	CD1	LEU	A	320	52.814	78.115	42.933	1.00	58.76
ATOM	2467	CD2	LEU	A	320	54.746	78.686	44.416	1.00	60.73
ATOM	2468	C	LEU	A	320	53.813	82.990	43.716	1.00	63.09
ATOM	2469	O	LEU	A	320	52.880	83.792	43.785	1.00	64.62
ATOM	2470	N	PRO	A	321	54.954	83.275	43.064	1.00	63.74
ATOM	2471	CD	PRO	A	321	56.192	82.471	43.116	1.00	62.83
ATOM	2472	CA	PRO	A	321	55.197	84.539	42.361	1.00	62.76
ATOM	2473	CB	PRO	A	321	56.714	84.559	42.218	1.00	62.57
ATOM	2474	CG	PRO	A	321	57.044	83.121	42.040	1.00	62.47
ATOM	2475	C	PRO	A	321	54.509	84.709	41.010	1.00	64.73
ATOM	2476	O	PRO	A	321	54.131	83.737	40.359	1.00	64.26
ATOM	2477	N	ASN	A	322	54.356	85.966	40.603	1.00	65.64
ATOM	2478	CA	ASN	A	322	53.752	86.314	39.319	1.00	65.62
ATOM	2479	CB	ASN	A	322	53.658	87.842	39.161	1.00	66.04
ATOM	2480	CG	ASN	A	322	52.356	88.423	39.688	1.00	68.38
ATOM	2481	OD1	ASN	A	322	51.273	88.121	39.178	1.00	68.67
ATOM	2482	ND2	ASN	A	322	52.457	89.277	40.701	1.00	69.07
ATOM	2483	C	ASN	A	322	54.697	85.797	38.250	1.00	64.31
ATOM	2484	O	ASN	A	322	55.853	85.489	38.534	1.00	64.17
ATOM	2485	N	MET	A	323	54.214	85.694	37.023	1.00	63.26
ATOM	2486	CA	MET	A	323	55.085	85.276	35.936	1.00	63.53
ATOM	2487	CB	MET	A	323	54.285	85.171	34.644	1.00	61.82
ATOM	2488	CG	MET	A	323	53.394	83.948	34.582	1.00	60.85
ATOM	2489	SD	MET	A	323	54.407	82.462	34.522	1.00	61.85
ATOM	2490	CE	MET	A	323	54.478	82.037	36.264	1.00	56.84
ATOM	2491	C	MET	A	323	56.115	86.404	35.827	1.00	65.41
ATOM	2492	O	MET	A	323	55.904	87.485	36.389	1.00	68.23
ATOM	2493	N	THR	A	324	57.229	86.177	35.140	1.00	63.28
ATOM	2494	CA	THR	A	324	58.212	87.244	35.021	1.00	61.50
ATOM	2495	CB	THR	A	324	59.634	86.737	34.758	1.00	60.94
ATOM	2496	OG1	THR	A	324	59.677	86.098	33.475	1.00	56.77
ATOM	2497	CG2	THR	A	324	60.092	85.794	35.860	1.00	59.11
ATOM	2498	C	THR	A	324	57.907	88.175	33.865	1.00	64.57
ATOM	2499	O	THR	A	324	57.150	87.843	32.947	1.00	62.76
ATOM	2500	N	GLN	A	325	58.517	89.352	33.932	1.00	66.88
ATOM	2501	CA	GLN	A	325	58.404	90.349	32.884	1.00	70.22
ATOM	2502	CB	GLN	A	325	59.038	91.663	33.352	1.00	73.91
ATOM	2503	CG	GLN	A	325	58.839	92.850	32.415	1.00	81.00
ATOM	2504	CD	GLN	A	325	59.394	92.606	31.025	1.00	83.18
ATOM	2505	OE1	GLN	A	325	60.568	92.255	30.859	1.00	84.56
ATOM	2506	NE2	GLN	A	325	58.551	92.798	30.011	1.00	86.43
ATOM	2507	C	GLN	A	325	59.270	89.691	31.825	1.00	68.86
ATOM	2508	O	GLN	A	325	60.394	89.285	32.107	1.00	70.31
ATOM	2509	N	GLY	A	326	58.773	89.563	30.610	1.00	68.73
ATOM	2510	CA	GLY	A	326	59.590	88.895	29.613	1.00	68.86
ATOM	2511	C	GLY	A	326	58.887	87.601	29.294	1.00	67.06
ATOM	2512	O	GLY	A	326	58.846	87.176	28.140	1.00	68.08
ATOM	2513	N	PHE	A	327	58.350	86.957	30.327	1.00	65.55
ATOM	2514	CA	PHE	A	327	57.578	85.753	30.101	1.00	64.38
ATOM	2515	CB	PHE	A	327	57.034	85.173	31.414	1.00	63.69
ATOM	2516	CG	PHE	A	327	55.843	84.276	31.218	1.00	62.82

146/396

Figure 2A-46

ATOM	2517	CD1	PHE	A	327	54.548	84.772	31.373	1.00	60.57
ATOM	2518	CD2	PHE	A	327	56.009	82.960	30.790	1.00	61.98
ATOM	2519	CE1	PHE	A	327	53.441	83.980	31.100	1.00	60.06
ATOM	2520	CE2	PHE	A	327	54.910	82.155	30.511	1.00	61.71
ATOM	2521	CZ	PHE	A	327	53.619	82.667	30.665	1.00	61.89
ATOM	2522	C	PHE	A	327	56.422	86.251	29.231	1.00	62.57
ATOM	2523	O	PHE	A	327	56.119	85.672	28.198	1.00	61.92
ATOM	2524	N	TRP	A	328	55.799	87.351	29.646	1.00	63.16
ATOM	2525	CA	TRP	A	328	54.690	87.933	28.885	1.00	66.79
ATOM	2526	CB	TRP	A	328	53.993	89.025	29.696	1.00	65.11
ATOM	2527	CG	TRP	A	328	53.270	88.517	30.895	1.00	62.58
ATOM	2528	CD2	TRP	A	328	52.051	87.765	30.906	1.00	62.45
ATOM	2529	CE2	TRP	A	328	51.735	87.502	32.257	1.00	63.35
ATOM	2530	CE3	TRP	A	328	51.193	87.288	29.906	1.00	60.39
ATOM	2531	CD1	TRP	A	328	53.636	88.672	32.197	1.00	61.21
ATOM	2532	NE1	TRP	A	328	52.719	88.068	33.024	1.00	62.62
ATOM	2533	CZ2	TRP	A	328	50.594	86.782	32.634	1.00	63.99
ATOM	2534	CZ3	TRP	A	328	50.059	86.574	30.279	1.00	58.59
ATOM	2535	CH2	TRP	A	328	49.770	86.329	31.630	1.00	62.18
ATOM	2536	C	TRP	A	328	55.128	88.523	27.543	1.00	67.94
ATOM	2537	O	TRP	A	328	54.368	88.510	26.569	1.00	67.12
ATOM	2538	N	GLU	A	329	56.354	89.036	27.493	1.00	70.74
ATOM	2539	CA	GLU	A	329	56.880	89.629	26.267	1.00	73.76
ATOM	2540	CB	GLU	A	329	57.996	90.623	26.598	1.00	77.53
ATOM	2541	CG	GLU	A	329	58.661	91.245	25.360	1.00	84.84
ATOM	2542	CD	GLU	A	329	57.772	92.256	24.623	1.00	87.93
ATOM	2543	OE1	GLU	A	329	56.542	92.024	24.509	1.00	88.46
ATOM	2544	OE2	GLU	A	329	58.316	93.280	24.143	1.00	89.69
ATOM	2545	C	GLU	A	329	57.409	88.601	25.270	1.00	74.14
ATOM	2546	O	GLU	A	329	57.128	88.679	24.073	1.00	76.21
ATOM	2547	N	ASN	A	330	58.165	87.630	25.766	1.00	73.72
ATOM	2548	CA	ASN	A	330	58.755	86.608	24.910	1.00	72.16
ATOM	2549	CB	ASN	A	330	60.040	86.101	25.555	1.00	71.53
ATOM	2550	CG	ASN	A	330	60.992	87.217	25.879	1.00	70.69
ATOM	2551	OD1	ASN	A	330	61.538	87.285	26.981	1.00	67.92
ATOM	2552	ND2	ASN	A	330	61.203	88.107	24.914	1.00	70.47
ATOM	2553	C	ASN	A	330	57.866	85.417	24.563	1.00	71.25
ATOM	2554	O	ASN	A	330	58.115	84.737	23.570	1.00	71.96
ATOM	2555	N	SER	A	331	56.844	85.157	25.375	1.00	71.16
ATOM	2556	CA	SER	A	331	55.945	84.024	25.138	1.00	71.48
ATOM	2557	CB	SER	A	331	55.007	83.795	26.339	1.00	70.64
ATOM	2558	OG	SER	A	331	55.652	83.206	27.451	1.00	68.18
ATOM	2559	C	SER	A	331	55.072	84.190	23.906	1.00	71.85
ATOM	2560	O	SER	A	331	54.609	85.289	23.599	1.00	73.54
ATOM	2561	N	MET	A	332	54.851	83.085	23.207	1.00	72.32
ATOM	2562	CA	MET	A	332	53.977	83.064	22.045	1.00	73.01
ATOM	2563	CB	MET	A	332	54.603	82.277	20.885	1.00	71.81
ATOM	2564	CG	MET	A	332	53.648	82.071	19.719	1.00	73.56
ATOM	2565	SD	MET	A	332	54.358	81.247	18.275	1.00	75.37
ATOM	2566	CE	MET	A	332	55.288	82.630	17.563	1.00	78.00
ATOM	2567	C	MET	A	332	52.728	82.342	22.547	1.00	73.62
ATOM	2568	O	MET	A	332	52.642	81.118	22.487	1.00	73.84
ATOM	2569	N	LEU	A	333	51.775	83.110	23.061	1.00	74.14
ATOM	2570	CA	LEU	A	333	50.532	82.568	23.598	1.00	75.70
ATOM	2571	CB	LEU	A	333	50.033	83.478	24.729	1.00	73.33
ATOM	2572	CG	LEU	A	333	50.560	83.254	26.153	1.00	74.98

147/396

Figure 2A-47

ATOM	2573	CD1	LEU	A	333	51.983	82.754	26.132	1.00	75.64
ATOM	2574	CD2	LEU	A	333	50.450	84.554	26.941	1.00	73.64
ATOM	2575	C	LEU	A	333	49.414	82.365	22.563	1.00	77.63
ATOM	2576	O	LEU	A	333	48.320	81.916	22.912	1.00	76.42
ATOM	2577	N	THR	A	334	49.688	82.692	21.300	1.00	81.01
ATOM	2578	CA	THR	A	334	48.703	82.545	20.214	1.00	82.62
ATOM	2579	CB	THR	A	334	47.935	83.868	19.957	1.00	82.72
ATOM	2580	OG1	THR	A	334	48.856	84.966	19.967	1.00	83.25
ATOM	2581	CG2	THR	A	334	46.870	84.096	21.021	1.00	83.11
ATOM	2582	C	THR	A	334	49.371	82.130	18.905	1.00	83.24
ATOM	2583	O	THR	A	334	50.539	82.431	18.681	1.00	83.49
ATOM	2584	N	ASP	A	335	48.635	81.438	18.041	1.00	85.97
ATOM	2585	CA	ASP	A	335	49.195	81.014	16.762	1.00	89.21
ATOM	2586	CB	ASP	A	335	48.287	79.979	16.082	1.00	89.68
ATOM	2587	CG	ASP	A	335	48.893	79.414	14.794	1.00	91.75
ATOM	2588	OD1	ASP	A	335	48.360	78.409	14.268	1.00	89.87
ATOM	2589	OD2	ASP	A	335	49.899	79.975	14.302	1.00	92.52
ATOM	2590	C	ASP	A	335	49.335	82.249	15.881	1.00	90.75
ATOM	2591	O	ASP	A	335	48.379	83.007	15.716	1.00	90.87
ATOM	2592	N	PRO	A	336	50.537	82.478	15.322	1.00	92.24
ATOM	2593	CD	PRO	A	336	51.782	81.751	15.614	1.00	92.46
ATOM	2594	CA	PRO	A	336	50.811	83.630	14.454	1.00	94.30
ATOM	2595	CB	PRO	A	336	52.316	83.533	14.214	1.00	93.93
ATOM	2596	CG	PRO	A	336	52.814	82.828	15.422	1.00	92.88
ATOM	2597	C	PRO	A	336	50.018	83.582	13.147	1.00	95.79
ATOM	2598	O	PRO	A	336	49.998	84.550	12.384	1.00	94.80
ATOM	2599	N	GLY	A	337	49.377	82.442	12.899	1.00	97.98
ATOM	2600	CA	GLY	A	337	48.578	82.271	11.699	1.00	99.28
ATOM	2601	C	GLY	A	337	49.354	81.732	10.513	1.00	101.17
ATOM	2602	O	GLY	A	337	50.170	80.813	10.645	1.00	101.21
ATOM	2603	N	ASN	A	338	49.091	82.315	9.347	1.00	102.32
ATOM	2604	CA	ASN	A	338	49.739	81.922	8.101	1.00	102.25
ATOM	2605	CB	ASN	A	338	48.791	82.189	6.925	1.00	103.07
ATOM	2606	CG	ASN	A	338	48.251	83.617	6.915	1.00	104.24
ATOM	2607	OD1	ASN	A	338	47.499	84.001	6.018	1.00	104.70
ATOM	2608	ND2	ASN	A	338	48.632	84.406	7.918	1.00	104.05
ATOM	2609	C	ASN	A	338	51.058	82.662	7.882	1.00	101.95
ATOM	2610	O	ASN	A	338	51.210	83.816	8.287	1.00	102.34
ATOM	2611	N	VAL	A	339	52.006	81.989	7.236	1.00	101.25
ATOM	2612	CA	VAL	A	339	53.317	82.570	6.954	1.00	101.33
ATOM	2613	CB	VAL	A	339	53.180	83.943	6.239	1.00	101.22
ATOM	2614	CG1	VAL	A	339	54.534	84.393	5.705	1.00	101.18
ATOM	2615	CG2	VAL	A	339	52.174	83.842	5.099	1.00	100.66
ATOM	2616	C	VAL	A	339	54.101	82.740	8.257	1.00	101.28
ATOM	2617	O	VAL	A	339	55.008	83.569	8.364	1.00	100.69
ATOM	2618	N	GLN	A	340	53.734	81.936	9.249	1.00	101.44
ATOM	2619	CA	GLN	A	340	54.378	81.951	10.558	1.00	99.82
ATOM	2620	CB	GLN	A	340	53.752	83.025	11.447	1.00	99.15
ATOM	2621	CG	GLN	A	340	54.463	84.369	11.415	1.00	96.42
ATOM	2622	CD	GLN	A	340	55.810	84.330	12.112	1.00	94.78
ATOM	2623	OE1	GLN	A	340	56.691	83.553	11.740	1.00	94.83
ATOM	2624	NE2	GLN	A	340	55.977	85.169	13.129	1.00	91.78
ATOM	2625	C	GLN	A	340	54.203	80.584	11.199	1.00	99.27
ATOM	2626	O	GLN	A	340	54.012	80.468	12.410	1.00	100.94
ATOM	2627	N	LYS	A	341	54.266	79.549	10.369	1.00	97.68
ATOM	2628	CA	LYS	A	341	54.118	78.181	10.837	1.00	97.73

148/396

Figure 2A-48

ATOM	2629	CB	LYS	A	341	54.473	77.205	9.709	1.00	98.08
ATOM	2630	CG	LYS	A	341	55.831	77.454	9.065	1.00	99.00
ATOM	2631	CD	LYS	A	341	56.050	76.598	7.814	1.00	99.05
ATOM	2632	CE	LYS	A	341	56.113	75.105	8.123	1.00	97.73
ATOM	2633	NZ	LYS	A	341	54.828	74.571	8.652	1.00	97.08
ATOM	2634	C	LYS	A	341	54.984	77.915	12.068	1.00	97.33
ATOM	2635	O	LYS	A	341	56.049	78.517	12.244	1.00	96.73
ATOM	2636	N	ALA	A	342	54.511	77.012	12.919	1.00	96.20
ATOM	2637	CA	ALA	A	342	55.213	76.657	14.144	1.00	94.29
ATOM	2638	CB	ALA	A	342	55.123	77.807	15.138	1.00	93.02
ATOM	2639	C	ALA	A	342	54.571	75.415	14.736	1.00	93.04
ATOM	2640	O	ALA	A	342	53.575	74.914	14.214	1.00	92.92
ATOM	2641	N	VAL	A	343	55.149	74.910	15.820	1.00	91.89
ATOM	2642	CA	VAL	A	343	54.588	73.748	16.493	1.00	90.62
ATOM	2643	CB	VAL	A	343	55.692	72.932	17.205	1.00	91.18
ATOM	2644	CG1	VAL	A	343	56.890	72.785	16.277	1.00	91.27
ATOM	2645	CG2	VAL	A	343	56.098	73.600	18.510	1.00	92.43
ATOM	2646	C	VAL	A	343	53.595	74.330	17.506	1.00	89.24
ATOM	2647	O	VAL	A	343	53.892	75.336	18.149	1.00	88.11
ATOM	2648	N	CYS	A	344	52.423	73.713	17.643	1.00	88.25
ATOM	2649	CA	CYS	A	344	51.399	74.230	18.551	1.00	86.17
ATOM	2650	C	CYS	A	344	51.011	73.405	19.771	1.00	83.62
ATOM	2651	O	CYS	A	344	51.338	72.224	19.873	1.00	82.66
ATOM	2652	CB	CYS	A	344	50.113	74.516	17.777	1.00	87.36
ATOM	2653	SG	CYS	A	344	50.081	76.047	16.799	1.00	87.61
ATOM	2654	N	HIS	A	345	50.288	74.073	20.676	1.00	81.97
ATOM	2655	CA	HIS	A	345	49.755	73.516	21.930	1.00	80.75
ATOM	2656	CB	HIS	A	345	48.490	72.686	21.645	1.00	85.30
ATOM	2657	CG	HIS	A	345	47.266	73.497	21.360	1.00	88.25
ATOM	2658	CD2	HIS	A	345	46.142	73.699	22.090	1.00	90.00
ATOM	2659	ND1	HIS	A	345	47.085	74.185	20.179	1.00	90.43
ATOM	2660	CE1	HIS	A	345	45.901	74.772	20.193	1.00	92.18
ATOM	2661	NE2	HIS	A	345	45.308	74.493	21.341	1.00	91.03
ATOM	2662	C	HIS	A	345	50.676	72.646	22.790	1.00	76.01
ATOM	2663	O	HIS	A	345	50.214	71.644	23.349	1.00	70.35
ATOM	2664	N	PRO	A	346	51.956	73.021	22.959	1.00	72.71
ATOM	2665	CD	PRO	A	346	52.967	73.268	21.923	1.00	70.39
ATOM	2666	CA	PRO	A	346	52.428	71.926	23.798	1.00	74.39
ATOM	2667	CB	PRO	A	346	52.783	70.892	22.744	1.00	76.15
ATOM	2668	CG	PRO	A	346	53.455	71.834	21.621	1.00	72.44
ATOM	2669	C	PRO	A	346	53.632	72.156	24.706	1.00	71.75
ATOM	2670	O	PRO	A	346	54.177	71.169	25.192	1.00	73.89
ATOM	2671	N	THR	A	347	54.064	73.387	24.975	1.00	66.04
ATOM	2672	CA	THR	A	347	55.298	73.478	25.745	1.00	62.85
ATOM	2673	CB	THR	A	347	56.492	73.327	24.783	1.00	62.28
ATOM	2674	OG1	THR	A	347	56.381	74.306	23.748	1.00	64.50
ATOM	2675	CG2	THR	A	347	56.521	71.940	24.145	1.00	60.57
ATOM	2676	C	THR	A	347	55.641	74.628	26.695	1.00	62.86
ATOM	2677	O	THR	A	347	55.272	75.784	26.476	1.00	61.54
ATOM	2678	N	ALA	A	348	56.383	74.273	27.748	1.00	59.80
ATOM	2679	CA	ALA	A	348	56.855	75.219	28.768	1.00	58.47
ATOM	2680	CB	ALA	A	348	56.418	74.766	30.161	1.00	53.83
ATOM	2681	C	ALA	A	348	58.376	75.238	28.668	1.00	55.36
ATOM	2682	O	ALA	A	348	59.016	74.190	28.712	1.00	56.29
ATOM	2683	N	TRP	A	349	58.964	76.419	28.534	1.00	54.93
ATOM	2684	CA	TRP	A	349	60.409	76.488	28.377	1.00	54.74

149/396

Figure 2A-49

ATOM	2685	CB	TRP	A	349	60.775	77.217	27.077	1.00	55.88
ATOM	2686	CG	TRP	A	349	60.248	76.618	25.808	1.00	56.38
ATOM	2687	CD2	TRP	A	349	61.005	76.304	24.630	1.00	54.12
ATOM	2688	CE2	TRP	A	349	60.087	75.863	23.650	1.00	55.24
ATOM	2689	CE3	TRP	A	349	62.368	76.359	24.307	1.00	56.29
ATOM	2690	CD1	TRP	A	349	58.941	76.355	25.503	1.00	55.42
ATOM	2691	NE1	TRP	A	349	58.838	75.904	24.211	1.00	56.06
ATOM	2692	CZ2	TRP	A	349	60.486	75.479	22.359	1.00	55.66
ATOM	2693	CZ3	TRP	A	349	62.770	75.981	23.024	1.00	58.52
ATOM	2694	CH2	TRP	A	349	61.826	75.546	22.063	1.00	59.12
ATOM	2695	C	TRP	A	349	61.193	77.148	29.495	1.00	53.74
ATOM	2696	O	TRP	A	349	60.789	78.170	30.052	1.00	56.09
ATOM	2697	N	ASP	A	350	62.338	76.548	29.785	1.00	54.63
ATOM	2698	CA	ASP	A	350	63.288	77.039	30.778	1.00	54.36
ATOM	2699	CB	ASP	A	350	63.484	75.992	31.887	1.00	54.70
ATOM	2700	CG	ASP	A	350	64.477	76.443	32.967	1.00	60.51
ATOM	2701	OD1	ASP	A	350	64.393	75.915	34.094	1.00	60.58
ATOM	2702	OD2	ASP	A	350	65.346	77.308	32.701	1.00	60.34
ATOM	2703	C	ASP	A	350	64.547	77.194	29.922	1.00	51.03
ATOM	2704	O	ASP	A	350	65.360	76.293	29.826	1.00	49.65
ATOM	2705	N	LEU	A	351	64.683	78.337	29.264	1.00	53.72
ATOM	2706	CA	LEU	A	351	65.820	78.556	28.375	1.00	55.92
ATOM	2707	CB	LEU	A	351	65.550	79.740	27.441	1.00	60.77
ATOM	2708	CG	LEU	A	351	64.339	79.614	26.514	1.00	62.45
ATOM	2709	CD1	LEU	A	351	63.084	80.023	27.275	1.00	63.69
ATOM	2710	CD2	LEU	A	351	64.530	80.509	25.287	1.00	63.91
ATOM	2711	C	LEU	A	351	67.144	78.772	29.067	1.00	55.49
ATOM	2712	O	LEU	A	351	68.200	78.572	28.472	1.00	58.07
ATOM	2713	N	GLY	A	352	67.089	79.174	30.326	1.00	53.93
ATOM	2714	CA	GLY	A	352	68.298	79.427	31.068	1.00	53.84
ATOM	2715	C	GLY	A	352	68.335	80.881	31.483	1.00	54.49
ATOM	2716	O	GLY	A	352	67.482	81.681	31.083	1.00	49.32
ATOM	2717	N	LYS	A	353	69.323	81.204	32.310	1.00	57.32
ATOM	2718	CA	LYS	A	353	69.537	82.553	32.814	1.00	59.47
ATOM	2719	CB	LYS	A	353	70.394	83.333	31.815	1.00	61.85
ATOM	2720	CG	LYS	A	353	70.873	84.687	32.331	1.00	70.30
ATOM	2721	CD	LYS	A	353	71.587	84.577	33.684	1.00	73.22
ATOM	2722	CE	LYS	A	353	72.034	85.957	34.184	1.00	75.24
ATOM	2723	NZ	LYS	A	353	70.896	86.924	34.288	1.00	72.65
ATOM	2724	C	LYS	A	353	68.253	83.324	33.137	1.00	59.82
ATOM	2725	O	LYS	A	353	68.073	84.470	32.702	1.00	60.70
ATOM	2726	N	GLY	A	354	67.367	82.691	33.907	1.00	58.15
ATOM	2727	CA	GLY	A	354	66.118	83.323	34.295	1.00	55.95
ATOM	2728	C	GLY	A	354	65.123	83.599	33.175	1.00	55.00
ATOM	2729	O	GLY	A	354	64.201	84.403	33.336	1.00	53.42
ATOM	2730	N	ASP	A	355	65.297	82.935	32.040	1.00	54.56
ATOM	2731	CA	ASP	A	355	64.407	83.130	30.900	1.00	53.53
ATOM	2732	CB	ASP	A	355	65.251	83.210	29.633	1.00	54.03
ATOM	2733	CG	ASP	A	355	64.448	83.595	28.408	1.00	57.86
ATOM	2734	OD1	ASP	A	355	65.083	83.938	27.391	1.00	63.59
ATOM	2735	OD2	ASP	A	355	63.200	83.554	28.446	1.00	58.20
ATOM	2736	C	ASP	A	355	63.375	81.990	30.802	1.00	53.76
ATOM	2737	O	ASP	A	355	63.708	80.853	30.460	1.00	52.77
ATOM	2738	N	PHE	A	356	62.122	82.304	31.106	1.00	54.88
ATOM	2739	CA	PHE	A	356	61.047	81.317	31.070	1.00	56.48
ATOM	2740	CB	PHE	A	356	60.394	81.211	32.451	1.00	52.73

150/396

Figure 2A-50

ATOM	2741	CG	PHE	A	356	61.376	80.983	33.560	1.00	56.69
ATOM	2742	CD1	PHE	A	356	61.920	82.058	34.260	1.00	53.32
ATOM	2743	CD2	PHE	A	356	61.809	79.690	33.871	1.00	55.28
ATOM	2744	CE1	PHE	A	356	62.889	81.850	35.260	1.00	55.74
ATOM	2745	CE2	PHE	A	356	62.774	79.471	34.863	1.00	54.60
ATOM	2746	CZ	PHE	A	356	63.317	80.551	35.559	1.00	53.53
ATOM	2747	C	PHE	A	356	60.001	81.717	30.042	1.00	57.12
ATOM	2748	O	PHE	A	356	59.652	82.888	29.944	1.00	56.36
ATOM	2749	N	ARG	A	357	59.496	80.749	29.281	1.00	57.02
ATOM	2750	CA	ARG	A	357	58.482	81.045	28.268	1.00	56.73
ATOM	2751	CB	ARG	A	357	59.128	81.387	26.923	1.00	55.05
ATOM	2752	CG	ARG	A	357	60.157	82.497	26.960	1.00	60.47
ATOM	2753	CD	ARG	A	357	60.769	82.736	25.586	1.00	58.48
ATOM	2754	NE	ARG	A	357	61.970	83.559	25.693	1.00	60.42
ATOM	2755	CZ	ARG	A	357	62.693	83.980	24.661	1.00	57.71
ATOM	2756	NH1	ARG	A	357	63.772	84.717	24.873	1.00	53.34
ATOM	2757	NH2	ARG	A	357	62.335	83.671	23.421	1.00	56.57
ATOM	2758	C	ARG	A	357	57.556	79.877	28.023	1.00	57.19
ATOM	2759	O	ARG	A	357	57.930	78.718	28.217	1.00	59.98
ATOM	2760	N	ILE	A	358	56.339	80.190	27.593	1.00	57.80
ATOM	2761	CA	ILE	A	358	55.371	79.161	27.231	1.00	55.52
ATOM	2762	CB	ILE	A	358	54.070	79.243	28.070	1.00	53.23
ATOM	2763	CG2	ILE	A	358	52.925	78.539	27.325	1.00	50.88
ATOM	2764	CG1	ILE	A	358	54.297	78.596	29.445	1.00	48.92
ATOM	2765	CD1	ILE	A	358	53.111	78.692	30.401	1.00	46.17
ATOM	2766	C	ILE	A	358	55.041	79.360	25.752	1.00	56.77
ATOM	2767	O	ILE	A	358	54.812	80.488	25.297	1.00	56.24
ATOM	2768	N	LEU	A	359	55.064	78.260	25.006	1.00	57.79
ATOM	2769	CA	LEU	A	359	54.746	78.248	23.586	1.00	57.17
ATOM	2770	CB	LEU	A	359	55.854	77.555	22.776	1.00	58.20
ATOM	2771	CG	LEU	A	359	55.514	77.070	21.350	1.00	61.04
ATOM	2772	CD1	LEU	A	359	54.708	78.110	20.590	1.00	59.93
ATOM	2773	CD2	LEU	A	359	56.798	76.756	20.604	1.00	59.20
ATOM	2774	C	LEU	A	359	53.457	77.462	23.465	1.00	60.57
ATOM	2775	O	LEU	A	359	53.421	76.267	23.764	1.00	59.61
ATOM	2776	N	MET	A	360	52.395	78.135	23.038	1.00	62.19
ATOM	2777	CA	MET	A	360	51.107	77.485	22.900	1.00	63.75
ATOM	2778	CB	MET	A	360	50.503	77.279	24.289	1.00	63.18
ATOM	2779	CG	MET	A	360	49.405	76.236	24.381	1.00	62.94
ATOM	2780	SD	MET	A	360	48.676	76.171	26.048	1.00	68.20
ATOM	2781	CE	MET	A	360	46.973	76.544	25.721	1.00	64.23
ATOM	2782	C	MET	A	360	50.178	78.348	22.047	1.00	67.15
ATOM	2783	O	MET	A	360	50.032	79.550	22.287	1.00	66.80
ATOM	2784	N	CYS	A	361	49.554	77.736	21.046	1.00	70.60
ATOM	2785	CA	CYS	A	361	48.624	78.464	20.184	1.00	74.09
ATOM	2786	C	CYS	A	361	47.275	78.341	20.872	1.00	74.09
ATOM	2787	O	CYS	A	361	46.424	77.548	20.478	1.00	74.02
ATOM	2788	CB	CYS	A	361	48.600	77.839	18.786	1.00	76.93
ATOM	2789	SG	CYS	A	361	50.289	77.522	18.178	1.00	82.65
ATOM	2790	N	THR	A	362	47.109	79.145	21.918	1.00	74.15
ATOM	2791	CA	THR	A	362	45.910	79.151	22.742	1.00	75.36
ATOM	2792	CB	THR	A	362	46.082	80.138	23.915	1.00	76.61
ATOM	2793	OG1	THR	A	362	47.315	79.865	24.593	1.00	77.92
ATOM	2794	CG2	THR	A	362	44.939	80.000	24.905	1.00	76.33
ATOM	2795	C	THR	A	362	44.593	79.465	22.034	1.00	76.52
ATOM	2796	O	THR	A	362	44.493	80.422	21.271	1.00	76.96

151/396

Figure 2A-51

ATOM	2797	N	LYS	A	363	43.589	78.637	22.309	1.00	76.99
ATOM	2798	CA	LYS	A	363	42.244	78.796	21.765	1.00	77.30
ATOM	2799	CB	LYS	A	363	41.783	77.513	21.076	1.00	78.25
ATOM	2800	CG	LYS	A	363	42.663	77.048	19.928	1.00	81.77
ATOM	2801	CD	LYS	A	363	42.181	75.691	19.413	1.00	83.51
ATOM	2802	CE	LYS	A	363	43.077	75.139	18.310	1.00	85.53
ATOM	2803	NZ	LYS	A	363	42.570	73.831	17.800	1.00	85.09
ATOM	2804	C	LYS	A	363	41.332	79.077	22.959	1.00	77.49
ATOM	2805	O	LYS	A	363	41.629	78.656	24.082	1.00	78.20
ATOM	2806	N	VAL	A	364	40.226	79.778	22.726	1.00	75.53
ATOM	2807	CA	VAL	A	364	39.301	80.107	23.804	1.00	74.79
ATOM	2808	CB	VAL	A	364	38.432	81.322	23.432	1.00	73.06
ATOM	2809	CG1	VAL	A	364	37.542	81.715	24.609	1.00	72.12
ATOM	2810	CG2	VAL	A	364	39.328	82.480	23.040	1.00	72.77
ATOM	2811	C	VAL	A	364	38.393	78.932	24.160	1.00	75.58
ATOM	2812	O	VAL	A	364	37.185	78.971	23.926	1.00	76.85
ATOM	2813	N	THR	A	365	38.985	77.893	24.738	1.00	75.00
ATOM	2814	CA	THR	A	365	38.248	76.701	25.129	1.00	73.31
ATOM	2815	CB	THR	A	365	38.658	75.511	24.265	1.00	74.35
ATOM	2816	OG1	THR	A	365	38.341	75.799	22.898	1.00	76.80
ATOM	2817	CG2	THR	A	365	37.920	74.243	24.697	1.00	78.32
ATOM	2818	C	THR	A	365	38.522	76.360	26.583	1.00	72.05
ATOM	2819	O	THR	A	365	39.474	76.865	27.176	1.00	70.89
ATOM	2820	N	MET	A	366	37.680	75.513	27.163	1.00	70.20
ATOM	2821	CA	MET	A	366	37.880	75.105	28.541	1.00	69.08
ATOM	2822	CB	MET	A	366	36.714	74.243	29.030	1.00	68.06
ATOM	2823	CG	MET	A	366	36.720	74.005	30.537	1.00	68.56
ATOM	2824	SD	MET	A	366	35.419	72.887	31.117	1.00	68.81
ATOM	2825	CE	MET	A	366	36.296	71.302	30.985	1.00	67.74
ATOM	2826	C	MET	A	366	39.170	74.294	28.566	1.00	67.85
ATOM	2827	O	MET	A	366	39.990	74.433	29.473	1.00	68.41
ATOM	2828	N	ASP	A	367	39.357	73.463	27.548	1.00	65.80
ATOM	2829	CA	ASP	A	367	40.548	72.635	27.467	1.00	65.93
ATOM	2830	CB	ASP	A	367	40.503	71.761	26.213	1.00	66.37
ATOM	2831	CG	ASP	A	367	39.584	70.552	26.374	1.00	69.79
ATOM	2832	OD1	ASP	A	367	38.834	70.487	27.378	1.00	67.88
ATOM	2833	OD2	ASP	A	367	39.609	69.668	25.490	1.00	71.49
ATOM	2834	C	ASP	A	367	41.854	73.421	27.501	1.00	66.37
ATOM	2835	O	ASP	A	367	42.797	73.018	28.178	1.00	67.46
ATOM	2836	N	ASP	A	368	41.920	74.541	26.786	1.00	65.15
ATOM	2837	CA	ASP	A	368	43.146	75.333	26.766	1.00	63.30
ATOM	2838	CB	ASP	A	368	43.196	76.204	25.513	1.00	63.36
ATOM	2839	CG	ASP	A	368	43.573	75.409	24.297	1.00	64.17
ATOM	2840	OD1	ASP	A	368	43.065	74.278	24.167	1.00	67.09
ATOM	2841	OD2	ASP	A	368	44.369	75.900	23.471	1.00	69.71
ATOM	2842	C	ASP	A	368	43.326	76.176	28.009	1.00	60.93
ATOM	2843	O	ASP	A	368	44.420	76.664	28.287	1.00	60.59
ATOM	2844	N	PHE	A	369	42.245	76.346	28.756	1.00	58.37
ATOM	2845	CA	PHE	A	369	42.292	77.101	29.996	1.00	57.96
ATOM	2846	CB	PHE	A	369	40.862	77.506	30.392	1.00	54.36
ATOM	2847	CG	PHE	A	369	40.704	77.923	31.836	1.00	56.81
ATOM	2848	CD1	PHE	A	369	40.382	76.983	32.817	1.00	53.92
ATOM	2849	CD2	PHE	A	369	40.820	79.258	32.205	1.00	56.60
ATOM	2850	CE1	PHE	A	369	40.174	77.364	34.139	1.00	52.25
ATOM	2851	CE2	PHE	A	369	40.612	79.655	33.530	1.00	59.26
ATOM	2852	CZ	PHE	A	369	40.286	78.701	34.499	1.00	58.16

152/396

Figure 2A-52

ATOM	2853	C	PHE	A	369	42.956	76.212	31.064	1.00	57.32
ATOM	2854	O	PHE	A	369	43.662	76.702	31.947	1.00	57.25
ATOM	2855	N	LEU	A	370	42.739	74.902	30.956	1.00	57.44
ATOM	2856	CA	LEU	A	370	43.307	73.936	31.894	1.00	56.64
ATOM	2857	CB	LEU	A	370	42.488	72.644	31.890	1.00	54.55
ATOM	2858	CG	LEU	A	370	41.008	72.821	32.220	1.00	55.54
ATOM	2859	CD1	LEU	A	370	40.267	71.514	31.987	1.00	52.69
ATOM	2860	CD2	LEU	A	370	40.863	73.299	33.662	1.00	55.28
ATOM	2861	C	LEU	A	370	44.744	73.626	31.508	1.00	56.64
ATOM	2862	O	LEU	A	370	45.597	73.421	32.374	1.00	57.19
ATOM	2863	N	THR	A	371	45.011	73.587	30.204	1.00	54.59
ATOM	2864	CA	THR	A	371	46.362	73.312	29.727	1.00	54.19
ATOM	2865	CB	THR	A	371	46.393	73.131	28.199	1.00	52.45
ATOM	2866	OG1	THR	A	371	45.805	71.872	27.863	1.00	51.88
ATOM	2867	CG2	THR	A	371	47.811	73.149	27.685	1.00	49.37
ATOM	2868	C	THR	A	371	47.294	74.449	30.132	1.00	54.47
ATOM	2869	O	THR	A	371	48.468	74.228	30.463	1.00	53.75
ATOM	2870	N	ALA	A	372	46.759	75.664	30.115	1.00	53.51
ATOM	2871	CA	ALA	A	372	47.526	76.837	30.502	1.00	53.29
ATOM	2872	CB	ALA	A	372	46.689	78.095	30.320	1.00	53.64
ATOM	2873	C	ALA	A	372	47.949	76.699	31.968	1.00	52.69
ATOM	2874	O	ALA	A	372	49.079	77.032	32.323	1.00	52.83
ATOM	2875	N	HIS	A	373	47.037	76.234	32.817	1.00	50.16
ATOM	2876	CA	HIS	A	373	47.351	76.055	34.227	1.00	50.32
ATOM	2877	CB	HIS	A	373	46.095	75.692	35.023	1.00	51.31
ATOM	2878	CG	HIS	A	373	45.195	76.856	35.292	1.00	53.60
ATOM	2879	CD2	HIS	A	373	45.011	77.598	36.410	1.00	54.22
ATOM	2880	ND1	HIS	A	373	44.354	77.387	34.338	1.00	56.48
ATOM	2881	CE1	HIS	A	373	43.690	78.405	34.857	1.00	55.71
ATOM	2882	NE2	HIS	A	373	44.070	78.554	36.113	1.00	54.41
ATOM	2883	C	HIS	A	373	48.394	74.946	34.361	1.00	51.28
ATOM	2884	O	HIS	A	373	49.397	75.093	35.070	1.00	49.56
ATOM	2885	N	HIS	A	374	48.158	73.835	33.666	1.00	49.07
ATOM	2886	CA	HIS	A	374	49.097	72.730	33.697	1.00	46.01
ATOM	2887	CB	HIS	A	374	48.636	71.621	32.744	1.00	41.04
ATOM	2888	CG	HIS	A	374	49.681	70.585	32.464	1.00	32.65
ATOM	2889	CD2	HIS	A	374	50.918	70.689	31.919	1.00	38.71
ATOM	2890	ND1	HIS	A	374	49.487	69.244	32.719	1.00	36.57
ATOM	2891	CE1	HIS	A	374	50.560	68.566	32.336	1.00	39.54
ATOM	2892	NE2	HIS	A	374	51.446	69.420	31.848	1.00	31.36
ATOM	2893	C	HIS	A	374	50.474	73.243	33.285	1.00	48.95
ATOM	2894	O	HIS	A	374	51.451	73.099	34.027	1.00	47.64
ATOM	2895	N	GLU	A	375	50.547	73.850	32.097	1.00	52.66
ATOM	2896	CA	GLU	A	375	51.810	74.362	31.589	1.00	51.50
ATOM	2897	CB	GLU	A	375	51.652	74.846	30.149	1.00	56.24
ATOM	2898	CG	GLU	A	375	51.364	73.721	29.140	1.00	62.39
ATOM	2899	CD	GLU	A	375	52.427	72.627	29.133	1.00	64.20
ATOM	2900	OE1	GLU	A	375	53.632	72.960	29.123	1.00	68.02
ATOM	2901	OE2	GLU	A	375	52.062	71.431	29.123	1.00	66.27
ATOM	2902	C	GLU	A	375	52.411	75.460	32.464	1.00	49.78
ATOM	2903	O	GLU	A	375	53.625	75.506	32.659	1.00	48.96
ATOM	2904	N	MET	A	376	51.594	76.351	33.005	1.00	46.83
ATOM	2905	CA	MET	A	376	52.189	77.360	33.858	1.00	47.72
ATOM	2906	CB	MET	A	376	51.191	78.464	34.201	1.00	49.34
ATOM	2907	CG	MET	A	376	51.843	79.676	34.870	1.00	51.23
ATOM	2908	SD	MET	A	376	50.699	81.052	35.138	1.00	57.92

153/396

Figure 2A-53

ATOM	2909	CE	MET	A	376	50.785	81.788	33.485	1.00	46.90
ATOM	2910	C	MET	A	376	52.677	76.678	35.138	1.00	49.00
ATOM	2911	O	MET	A	376	53.458	77.251	35.886	1.00	51.22
ATOM	2912	N	GLY	A	377	52.206	75.455	35.388	1.00	50.99
ATOM	2913	CA	GLY	A	377	52.622	74.721	36.571	1.00	46.56
ATOM	2914	C	GLY	A	377	54.082	74.354	36.422	1.00	46.15
ATOM	2915	O	GLY	A	377	54.854	74.388	37.383	1.00	45.81
ATOM	2916	N	HIS	A	378	54.459	74.000	35.199	1.00	43.25
ATOM	2917	CA	HIS	A	378	55.832	73.649	34.877	1.00	43.54
ATOM	2918	CB	HIS	A	378	55.944	73.195	33.434	1.00	46.17
ATOM	2919	CG	HIS	A	378	55.380	71.842	33.173	1.00	50.88
ATOM	2920	CD2	HIS	A	378	54.483	71.415	32.255	1.00	49.13
ATOM	2921	ND1	HIS	A	378	55.833	70.714	33.822	1.00	51.09
ATOM	2922	CE1	HIS	A	378	55.246	69.649	33.309	1.00	47.67
ATOM	2923	NE2	HIS	A	378	54.424	70.048	32.356	1.00	50.04
ATOM	2924	C	HIS	A	378	56.788	74.829	35.038	1.00	44.17
ATOM	2925	O	HIS	A	378	57.927	74.669	35.485	1.00	40.16
ATOM	2926	N	ILE	A	379	56.340	76.001	34.603	1.00	43.76
ATOM	2927	CA	ILE	A	379	57.162	77.197	34.686	1.00	46.58
ATOM	2928	CB	ILE	A	379	56.420	78.411	34.080	1.00	46.24
ATOM	2929	CG2	ILE	A	379	57.274	79.674	34.241	1.00	45.15
ATOM	2930	CG1	ILE	A	379	56.114	78.150	32.601	1.00	42.51
ATOM	2931	CD1	ILE	A	379	57.358	78.046	31.717	1.00	41.84
ATOM	2932	C	ILE	A	379	57.476	77.475	36.157	1.00	47.63
ATOM	2933	O	ILE	A	379	58.629	77.698	36.552	1.00	47.19
ATOM	2934	N	GLN	A	380	56.420	77.431	36.953	1.00	47.10
ATOM	2935	CA	GLN	A	380	56.492	77.668	38.377	1.00	49.52
ATOM	2936	CB	GLN	A	380	55.132	77.351	38.985	1.00	51.57
ATOM	2937	CG	GLN	A	380	54.863	78.079	40.248	1.00	55.42
ATOM	2938	CD	GLN	A	380	54.750	79.558	40.014	1.00	57.78
ATOM	2939	OE1	GLN	A	380	55.321	80.345	40.750	1.00	59.72
ATOM	2940	NE2	GLN	A	380	54.001	79.948	38.987	1.00	58.20
ATOM	2941	C	GLN	A	380	57.565	76.776	38.996	1.00	50.85
ATOM	2942	O	GLN	A	380	58.387	77.222	39.805	1.00	52.22
ATOM	2943	N	TYR	A	381	57.550	75.513	38.596	1.00	48.82
ATOM	2944	CA	TYR	A	381	58.491	74.538	39.097	1.00	48.10
ATOM	2945	CB	TYR	A	381	58.097	73.143	38.590	1.00	46.22
ATOM	2946	CG	TYR	A	381	58.705	71.955	39.318	1.00	43.24
ATOM	2947	CD1	TYR	A	381	58.187	70.666	39.119	1.00	44.44
ATOM	2948	CE1	TYR	A	381	58.721	69.551	39.779	1.00	46.00
ATOM	2949	CD2	TYR	A	381	59.782	72.105	40.198	1.00	39.71
ATOM	2950	CE2	TYR	A	381	60.329	70.996	40.866	1.00	41.56
ATOM	2951	CZ	TYR	A	381	59.792	69.722	40.648	1.00	43.31
ATOM	2952	OH	TYR	A	381	60.340	68.618	41.246	1.00	37.97
ATOM	2953	C	TYR	A	381	59.879	74.927	38.618	1.00	46.38
ATOM	2954	O	TYR	A	381	60.847	74.810	39.362	1.00	49.50
ATOM	2955	N	ASP	A	382	59.980	75.400	37.383	1.00	46.40
ATOM	2956	CA	ASP	A	382	61.266	75.817	36.834	1.00	46.71
ATOM	2957	CB	ASP	A	382	61.122	76.179	35.362	1.00	52.07
ATOM	2958	CG	ASP	A	382	60.775	74.991	34.495	1.00	53.20
ATOM	2959	OD1	ASP	A	382	61.370	73.906	34.690	1.00	52.04
ATOM	2960	OD2	ASP	A	382	59.920	75.159	33.599	1.00	57.81
ATOM	2961	C	ASP	A	382	61.825	77.040	37.574	1.00	47.93
ATOM	2962	O	ASP	A	382	63.033	77.146	37.819	1.00	45.62
ATOM	2963	N	MET	A	383	60.940	77.970	37.910	1.00	46.73
ATOM	2964	CA	MET	A	383	61.342	79.175	38.610	1.00	48.86

154/396

Figure 2A-54

ATOM	2965	CB	MET	A	383	60.189	80.178	38.624	1.00	48.28
ATOM	2966	CG	MET	A	383	59.866	80.753	37.245	1.00	50.55
ATOM	2967	SD	MET	A	383	58.323	81.665	37.251	1.00	57.89
ATOM	2968	CE	MET	A	383	58.618	82.863	38.530	1.00	52.99
ATOM	2969	C	MET	A	383	61.779	78.868	40.034	1.00	49.61
ATOM	2970	O	MET	A	383	62.776	79.409	40.513	1.00	53.33
ATOM	2971	N	ALA	A	384	61.042	77.986	40.698	1.00	48.72
ATOM	2972	CA	ALA	A	384	61.340	77.621	42.074	1.00	47.67
ATOM	2973	CB	ALA	A	384	60.277	76.635	42.593	1.00	43.89
ATOM	2974	C	ALA	A	384	62.743	77.049	42.278	1.00	47.43
ATOM	2975	O	ALA	A	384	63.353	77.264	43.320	1.00	50.35
ATOM	2976	N	TYR	A	385	63.270	76.326	41.298	1.00	46.48
ATOM	2977	CA	TYR	A	385	64.605	75.758	41.457	1.00	45.24
ATOM	2978	CB	TYR	A	385	64.563	74.235	41.227	1.00	46.65
ATOM	2979	CG	TYR	A	385	64.076	73.757	39.864	1.00	44.15
ATOM	2980	CD1	TYR	A	385	63.212	72.665	39.773	1.00	45.98
ATOM	2981	CE1	TYR	A	385	62.848	72.109	38.537	1.00	45.16
ATOM	2982	CD2	TYR	A	385	64.563	74.304	38.670	1.00	44.79
ATOM	2983	CE2	TYR	A	385	64.202	73.748	37.414	1.00	45.32
ATOM	2984	CZ	TYR	A	385	63.345	72.642	37.370	1.00	45.81
ATOM	2985	OH	TYR	A	385	63.019	72.026	36.176	1.00	47.59
ATOM	2986	C	TYR	A	385	65.682	76.391	40.574	1.00	43.75
ATOM	2987	O	TYR	A	385	66.740	75.804	40.361	1.00	41.01
ATOM	2988	N	ALA	A	386	65.412	77.588	40.063	1.00	43.21
ATOM	2989	CA	ALA	A	386	66.370	78.270	39.202	1.00	46.73
ATOM	2990	CB	ALA	A	386	65.763	79.561	38.682	1.00	45.36
ATOM	2991	C	ALA	A	386	67.711	78.559	39.888	1.00	50.22
ATOM	2992	O	ALA	A	386	68.745	78.625	39.221	1.00	52.83
ATOM	2993	N	ALA	A	387	67.706	78.707	41.213	1.00	50.72
ATOM	2994	CA	ALA	A	387	68.939	79.005	41.950	1.00	51.61
ATOM	2995	CB	ALA	A	387	68.607	79.592	43.312	1.00	51.13
ATOM	2996	C	ALA	A	387	69.847	77.800	42.124	1.00	53.18
ATOM	2997	O	ALA	A	387	71.025	77.942	42.468	1.00	55.78
ATOM	2998	N	GLN	A	388	69.305	76.609	41.912	1.00	51.45
ATOM	2999	CA	GLN	A	388	70.105	75.393	42.045	1.00	49.32
ATOM	3000	CB	GLN	A	388	69.199	74.163	41.914	1.00	49.37
ATOM	3001	CG	GLN	A	388	68.173	73.995	43.029	1.00	48.61
ATOM	3002	CD	GLN	A	388	68.798	73.571	44.347	1.00	49.68
ATOM	3003	OE1	GLN	A	388	69.818	72.887	44.365	1.00	50.26
ATOM	3004	NE2	GLN	A	388	68.169	73.951	45.458	1.00	49.11
ATOM	3005	C	GLN	A	388	71.145	75.365	40.929	1.00	49.26
ATOM	3006	O	GLN	A	388	70.984	76.035	39.915	1.00	51.07
ATOM	3007	N	PRO	A	389	72.251	74.631	41.112	1.00	49.06
ATOM	3008	CD	PRO	A	389	72.838	74.007	42.307	1.00	47.67
ATOM	3009	CA	PRO	A	389	73.198	74.627	39.994	1.00	49.09
ATOM	3010	CB	PRO	A	389	74.397	73.852	40.540	1.00	47.08
ATOM	3011	CG	PRO	A	389	73.828	73.062	41.695	1.00	50.00
ATOM	3012	C	PRO	A	389	72.556	73.937	38.771	1.00	50.36
ATOM	3013	O	PRO	A	389	71.662	73.101	38.913	1.00	46.70
ATOM	3014	N	PHE	A	390	73.029	74.309	37.587	1.00	48.83
ATOM	3015	CA	PHE	A	390	72.541	73.798	36.316	1.00	49.69
ATOM	3016	CB	PHE	A	390	73.618	73.989	35.251	1.00	50.06
ATOM	3017	CG	PHE	A	390	73.158	73.656	33.873	1.00	49.76
ATOM	3018	CD1	PHE	A	390	72.525	74.612	33.093	1.00	51.81
ATOM	3019	CD2	PHE	A	390	73.318	72.371	33.369	1.00	49.34
ATOM	3020	CE1	PHE	A	390	72.051	74.291	31.818	1.00	55.16

155/396

Figure 2A-55

ATOM	3021	CE2	PHE	A	390	72.850	72.037	32.103	1.00	52.21
ATOM	3022	CZ	PHE	A	390	72.214	72.999	31.325	1.00	54.00
ATOM	3023	C	PHE	A	390	72.076	72.338	36.279	1.00	48.10
ATOM	3024	O	PHE	A	390	70.940	72.045	35.891	1.00	43.62
ATOM	3025	N	LEU	A	391	72.971	71.431	36.654	1.00	48.94
ATOM	3026	CA	LEU	A	391	72.685	69.999	36.642	1.00	48.42
ATOM	3027	CB	LEU	A	391	73.972	69.205	36.868	1.00	47.09
ATOM	3028	CG	LEU	A	391	74.922	69.184	35.673	1.00	48.72
ATOM	3029	CD1	LEU	A	391	76.307	68.724	36.104	1.00	43.97
ATOM	3030	CD2	LEU	A	391	74.344	68.283	34.585	1.00	40.57
ATOM	3031	C	LEU	A	391	71.627	69.534	37.634	1.00	49.36
ATOM	3032	O	LEU	A	391	71.124	68.407	37.513	1.00	51.55
ATOM	3033	N	LEU	A	392	71.275	70.380	38.601	1.00	45.11
ATOM	3034	CA	LEU	A	392	70.264	70.000	39.584	1.00	42.56
ATOM	3035	CB	LEU	A	392	70.729	70.374	40.996	1.00	46.49
ATOM	3036	CG	LEU	A	392	71.575	69.352	41.755	1.00	50.09
ATOM	3037	CD1	LEU	A	392	72.285	68.414	40.803	1.00	46.06
ATOM	3038	CD2	LEU	A	392	72.561	70.096	42.658	1.00	49.49
ATOM	3039	C	LEU	A	392	68.919	70.650	39.305	1.00	41.43
ATOM	3040	O	LEU	A	392	67.984	70.532	40.100	1.00	38.53
ATOM	3041	N	ARG	A	393	68.821	71.349	38.182	1.00	41.45
ATOM	3042	CA	ARG	A	393	67.569	71.997	37.835	1.00	44.47
ATOM	3043	CB	ARG	A	393	67.819	73.267	37.025	1.00	46.00
ATOM	3044	CG	ARG	A	393	68.572	74.358	37.738	1.00	49.46
ATOM	3045	CD	ARG	A	393	68.587	75.593	36.865	1.00	52.77
ATOM	3046	NE	ARG	A	393	69.776	76.398	37.094	1.00	56.98
ATOM	3047	CZ	ARG	A	393	70.291	77.229	36.197	1.00	60.02
ATOM	3048	NH1	ARG	A	393	69.721	77.364	35.005	1.00	56.24
ATOM	3049	NH2	ARG	A	393	71.382	77.924	36.492	1.00	63.37
ATOM	3050	C	ARG	A	393	66.667	71.060	37.028	1.00	45.10
ATOM	3051	O	ARG	A	393	66.710	71.043	35.796	1.00	42.04
ATOM	3052	N	ASN	A	394	65.864	70.281	37.739	1.00	45.95
ATOM	3053	CA	ASN	A	394	64.927	69.357	37.125	1.00	48.40
ATOM	3054	CB	ASN	A	394	65.674	68.225	36.431	1.00	51.37
ATOM	3055	CG	ASN	A	394	64.909	67.677	35.227	1.00	58.19
ATOM	3056	OD1	ASN	A	394	65.498	67.073	34.332	1.00	59.65
ATOM	3057	ND2	ASN	A	394	63.592	67.878	35.209	1.00	53.00
ATOM	3058	C	ASN	A	394	64.036	68.817	38.236	1.00	48.78
ATOM	3059	O	ASN	A	394	64.245	69.148	39.407	1.00	46.30
ATOM	3060	N	GLY	A	395	63.028	68.023	37.878	1.00	44.70
ATOM	3061	CA	GLY	A	395	62.154	67.462	38.896	1.00	44.94
ATOM	3062	C	GLY	A	395	62.920	66.461	39.754	1.00	42.83
ATOM	3063	O	GLY	A	395	63.915	65.909	39.287	1.00	40.79
ATOM	3064	N	ALA	A	396	62.467	66.225	40.990	1.00	43.06
ATOM	3065	CA	ALA	A	396	63.132	65.271	41.900	1.00	40.44
ATOM	3066	CB	ALA	A	396	62.255	64.998	43.119	1.00	38.16
ATOM	3067	C	ALA	A	396	63.453	63.983	41.150	1.00	42.07
ATOM	3068	O	ALA	A	396	64.555	63.438	41.281	1.00	45.39
ATOM	3069	N	ASN	A	397	62.484	63.466	40.394	1.00	41.89
ATOM	3070	CA	ASN	A	397	62.734	62.313	39.531	1.00	39.11
ATOM	3071	CB	ASN	A	397	62.616	60.958	40.282	1.00	42.20
ATOM	3072	CG	ASN	A	397	61.205	60.577	40.661	1.00	44.80
ATOM	3073	OD1	ASN	A	397	60.999	59.926	41.702	1.00	46.05
ATOM	3074	ND2	ASN	A	397	60.231	60.935	39.830	1.00	34.08
ATOM	3075	C	ASN	A	397	61.845	62.404	38.280	1.00	37.74
ATOM	3076	O	ASN	A	397	61.030	63.313	38.172	1.00	31.31

156/396

Figure 2A-56

ATOM	3077	N	GLU	A	398	62.022	61.477	37.342	1.00	38.28
ATOM	3078	CA	GLU	A	398	61.291	61.492	36.074	1.00	39.03
ATOM	3079	CB	GLU	A	398	61.547	60.190	35.295	1.00	37.42
ATOM	3080	CG	GLU	A	398	61.099	58.902	35.990	1.00	38.00
ATOM	3081	CD	GLU	A	398	61.341	57.678	35.128	1.00	44.07
ATOM	3082	OE1	GLU	A	398	62.268	57.700	34.292	1.00	48.52
ATOM	3083	OE2	GLU	A	398	60.618	56.676	35.283	1.00	49.43
ATOM	3084	C	GLU	A	398	59.801	61.760	36.163	1.00	41.69
ATOM	3085	O	GLU	A	398	59.214	62.356	35.259	1.00	45.76
ATOM	3086	N	GLY	A	399	59.193	61.395	37.280	1.00	43.60
ATOM	3087	CA	GLY	A	399	57.766	61.589	37.422	1.00	37.95
ATOM	3088	C	GLY	A	399	57.213	62.775	38.171	1.00	38.33
ATOM	3089	O	GLY	A	399	56.000	62.857	38.282	1.00	38.38
ATOM	3090	N	PHE	A	400	58.048	63.690	38.671	1.00	38.57
ATOM	3091	CA	PHE	A	400	57.546	64.870	39.433	1.00	38.46
ATOM	3092	CB	PHE	A	400	58.679	65.448	40.321	1.00	41.95
ATOM	3093	CG	PHE	A	400	58.796	64.809	41.705	1.00	45.08
ATOM	3094	CD1	PHE	A	400	58.923	63.429	41.855	1.00	44.99
ATOM	3095	CD2	PHE	A	400	58.811	65.609	42.854	1.00	42.27
ATOM	3096	CE1	PHE	A	400	59.065	62.849	43.134	1.00	46.58
ATOM	3097	CE2	PHE	A	400	58.955	65.041	44.141	1.00	42.52
ATOM	3098	CZ	PHE	A	400	59.081	63.662	44.278	1.00	41.99
ATOM	3099	C	PHE	A	400	56.934	66.060	38.629	1.00	34.66
ATOM	3100	O	PHE	A	400	55.889	66.590	38.998	1.00	36.31
ATOM	3101	N	HIS	A	401	57.604	66.496	37.561	1.00	36.04
ATOM	3102	CA	HIS	A	401	57.149	67.642	36.756	1.00	38.10
ATOM	3103	CB	HIS	A	401	58.115	67.865	35.559	1.00	36.58
ATOM	3104	CG	HIS	A	401	58.830	69.184	35.593	1.00	37.96
ATOM	3105	CD2	HIS	A	401	60.135	69.487	35.796	1.00	35.92
ATOM	3106	ND1	HIS	A	401	58.176	70.391	35.451	1.00	37.77
ATOM	3107	CE1	HIS	A	401	59.044	71.379	35.568	1.00	39.97
ATOM	3108	NE2	HIS	A	401	60.241	70.858	35.778	1.00	41.06
ATOM	3109	C	HIS	A	401	55.706	67.491	36.255	1.00	37.69
ATOM	3110	O	HIS	A	401	54.878	68.390	36.455	1.00	38.32
ATOM	3111	N	GLU	A	402	55.392	66.363	35.621	1.00	34.76
ATOM	3112	CA	GLU	A	402	54.027	66.167	35.143	1.00	40.97
ATOM	3113	CB	GLU	A	402	53.956	64.976	34.170	1.00	41.60
ATOM	3114	CG	GLU	A	402	54.650	65.278	32.840	1.00	42.31
ATOM	3115	CD	GLU	A	402	54.000	66.446	32.102	1.00	45.48
ATOM	3116	OE1	GLU	A	402	54.702	67.154	31.347	1.00	45.18
ATOM	3117	OE2	GLU	A	402	52.777	66.654	32.261	1.00	47.45
ATOM	3118	C	GLU	A	402	53.044	65.990	36.296	1.00	41.70
ATOM	3119	O	GLU	A	402	51.873	66.345	36.174	1.00	44.37
ATOM	3120	N	ALA	A	403	53.492	65.443	37.422	1.00	41.12
ATOM	3121	CA	ALA	A	403	52.569	65.305	38.551	1.00	41.75
ATOM	3122	CB	ALA	A	403	53.229	64.549	39.722	1.00	42.93
ATOM	3123	C	ALA	A	403	52.197	66.717	38.985	1.00	40.42
ATOM	3124	O	ALA	A	403	51.036	67.002	39.294	1.00	40.93
ATOM	3125	N	VAL	A	404	53.191	67.604	39.009	1.00	40.52
ATOM	3126	CA	VAL	A	404	52.955	68.995	39.397	1.00	42.39
ATOM	3127	CB	VAL	A	404	54.298	69.766	39.504	1.00	43.91
ATOM	3128	CG1	VAL	A	404	54.043	71.284	39.601	1.00	42.05
ATOM	3129	CG2	VAL	A	404	55.072	69.264	40.745	1.00	43.89
ATOM	3130	C	VAL	A	404	52.025	69.688	38.387	1.00	43.74
ATOM	3131	O	VAL	A	404	51.114	70.447	38.759	1.00	41.22
ATOM	3132	N	GLY	A	405	52.256	69.414	37.107	1.00	43.98

157/396

Figure 2A-57

ATOM	3133	CA	GLY	A	405	51.415	69.999	36.081	1.00	46.32
ATOM	3134	C	GLY	A	405	49.969	69.533	36.156	1.00	44.75
ATOM	3135	O	GLY	A	405	49.056	70.362	36.089	1.00	44.56
ATOM	3136	N	GLU	A	406	49.762	68.220	36.296	1.00	43.00
ATOM	3137	CA	GLU	A	406	48.418	67.629	36.375	1.00	44.66
ATOM	3138	CB	GLU	A	406	48.510	66.103	36.464	1.00	45.92
ATOM	3139	CG	GLU	A	406	49.040	65.410	35.223	1.00	49.54
ATOM	3140	CD	GLU	A	406	48.066	65.445	34.055	1.00	54.52
ATOM	3141	OE1	GLU	A	406	46.856	65.666	34.280	1.00	53.10
ATOM	3142	OE2	GLU	A	406	48.514	65.233	32.907	1.00	58.79
ATOM	3143	C	GLU	A	406	47.619	68.137	37.570	1.00	46.95
ATOM	3144	O	GLU	A	406	46.391	68.265	37.524	1.00	46.41
ATOM	3145	N	ILE	A	407	48.326	68.404	38.655	1.00	48.90
ATOM	3146	CA	ILE	A	407	47.712	68.903	39.874	1.00	51.60
ATOM	3147	CB	ILE	A	407	48.810	69.101	40.958	1.00	55.48
ATOM	3148	CG2	ILE	A	407	48.349	70.037	42.037	1.00	57.15
ATOM	3149	CG1	ILE	A	407	49.231	67.735	41.496	1.00	56.86
ATOM	3150	CD1	ILE	A	407	48.079	66.846	41.813	1.00	56.23
ATOM	3151	C	ILE	A	407	46.986	70.226	39.638	1.00	51.18
ATOM	3152	O	ILE	A	407	45.906	70.455	40.164	1.00	52.61
ATOM	3153	N	MET	A	408	47.586	71.102	38.845	1.00	49.59
ATOM	3154	CA	MET	A	408	46.989	72.397	38.591	1.00	49.25
ATOM	3155	CB	MET	A	408	47.995	73.281	37.846	1.00	49.46
ATOM	3156	CG	MET	A	408	49.335	73.392	38.552	1.00	47.20
ATOM	3157	SD	MET	A	408	49.145	73.527	40.349	1.00	57.52
ATOM	3158	CE	MET	A	408	50.781	73.062	40.908	1.00	51.18
ATOM	3159	C	MET	A	408	45.649	72.330	37.847	1.00	50.53
ATOM	3160	O	MET	A	408	44.735	73.082	38.167	1.00	51.76
ATOM	3161	N	SER	A	409	45.522	71.426	36.879	1.00	49.93
ATOM	3162	CA	SER	A	409	44.273	71.298	36.128	1.00	54.87
ATOM	3163	CB	SER	A	409	44.428	70.333	34.950	1.00	55.95
ATOM	3164	OG	SER	A	409	45.528	70.685	34.145	1.00	57.58
ATOM	3165	C	SER	A	409	43.177	70.766	37.031	1.00	56.08
ATOM	3166	O	SER	A	409	42.007	71.147	36.899	1.00	57.66
ATOM	3167	N	LEU	A	410	43.556	69.871	37.939	1.00	55.55
ATOM	3168	CA	LEU	A	410	42.602	69.283	38.864	1.00	54.11
ATOM	3169	CB	LEU	A	410	43.334	68.388	39.863	1.00	55.43
ATOM	3170	CG	LEU	A	410	42.852	66.939	40.004	1.00	57.73
ATOM	3171	CD1	LEU	A	410	42.720	66.275	38.631	1.00	51.01
ATOM	3172	CD2	LEU	A	410	43.828	66.181	40.891	1.00	56.06
ATOM	3173	C	LEU	A	410	41.837	70.393	39.586	1.00	55.17
ATOM	3174	O	LEU	A	410	40.615	70.456	39.503	1.00	58.82
ATOM	3175	N	SER	A	411	42.548	71.287	40.265	1.00	53.11
ATOM	3176	CA	SER	A	411	41.895	72.385	40.981	1.00	52.52
ATOM	3177	CB	SER	A	411	42.928	73.187	41.781	1.00	49.50
ATOM	3178	OG	SER	A	411	43.264	72.551	42.995	1.00	55.30
ATOM	3179	C	SER	A	411	41.139	73.364	40.075	1.00	51.63
ATOM	3180	O	SER	A	411	40.076	73.878	40.432	1.00	51.35
ATOM	3181	N	ALA	A	412	41.708	73.626	38.907	1.00	51.47
ATOM	3182	CA	ALA	A	412	41.143	74.577	37.962	1.00	51.68
ATOM	3183	CB	ALA	A	412	42.177	74.891	36.894	1.00	53.62
ATOM	3184	C	ALA	A	412	39.827	74.136	37.319	1.00	51.99
ATOM	3185	O	ALA	A	412	38.996	74.973	36.975	1.00	48.95
ATOM	3186	N	ALA	A	413	39.629	72.831	37.172	1.00	52.35
ATOM	3187	CA	ALA	A	413	38.397	72.319	36.573	1.00	53.94
ATOM	3188	CB	ALA	A	413	38.676	71.00 8	35.849	1.00	49.85

158/396

Figure 2A-58

ATOM	3189	C	ALA	A	413	37.230	72.127	37.553	1.00	55.45
ATOM	3190	O	ALA	A	413	36.080	72.017	37.131	1.00	55.34
ATOM	3191	N	THR	A	414	37.504	72.084	38.853	1.00	56.33
ATOM	3192	CA	THR	A	414	36.420	71.883	39.813	1.00	55.90
ATOM	3193	CB	THR	A	414	36.909	72.012	41.269	1.00	52.56
ATOM	3194	OG1	THR	A	414	37.376	73.346	41.500	1.00	54.24
ATOM	3195	CG2	THR	A	414	38.025	71.025	41.546	1.00	47.84
ATOM	3196	C	THR	A	414	35.290	72.889	39.615	1.00	59.77
ATOM	3197	O	THR	A	414	35.530	74.064	39.327	1.00	60.66
ATOM	3198	N	PRO	A	415	34.037	72.445	39.779	1.00	61.98
ATOM	3199	CD	PRO	A	415	33.599	71.086	40.133	1.00	62.93
ATOM	3200	CA	PRO	A	415	32.885	73.334	39.619	1.00	65.43
ATOM	3201	CB	PRO	A	415	31.724	72.462	40.080	1.00	65.39
ATOM	3202	CG	PRO	A	415	32.172	71.091	39.689	1.00	61.98
ATOM	3203	C	PRO	A	415	33.043	74.580	40.489	1.00	67.94
ATOM	3204	O	PRO	A	415	32.726	75.696	40.077	1.00	70.59
ATOM	3205	N	LYS	A	416	33.552	74.371	41.696	1.00	69.78
ATOM	3206	CA	LYS	A	416	33.753	75.445	42.655	1.00	70.11
ATOM	3207	CB	LYS	A	416	34.236	74.844	43.974	1.00	73.34
ATOM	3208	CG	LYS	A	416	34.380	75.816	45.128	1.00	76.33
ATOM	3209	CD	LYS	A	416	34.674	75.058	46.421	1.00	79.05
ATOM	3210	CE	LYS	A	416	35.907	74.162	46.278	1.00	79.75
ATOM	3211	NZ	LYS	A	416	36.185	73.427	47.543	1.00	83.09
ATOM	3212	C	LYS	A	416	34.738	76.497	42.159	1.00	70.66
ATOM	3213	O	LYS	A	416	34.573	77.689	42.428	1.00	71.00
ATOM	3214	N	HIS	A	417	35.766	76.068	41.436	1.00	69.58
ATOM	3215	CA	HIS	A	417	36.741	77.024	40.938	1.00	66.60
ATOM	3216	CB	HIS	A	417	38.003	76.323	40.455	1.00	63.05
ATOM	3217	CG	HIS	A	417	39.099	77.272	40.089	1.00	59.72
ATOM	3218	CD2	HIS	A	417	39.526	77.719	38.884	1.00	56.71
ATOM	3219	ND1	HIS	A	417	39.839	77.951	41.035	1.00	61.00
ATOM	3220	CE1	HIS	A	417	40.673	78.777	40.427	1.00	58.28
ATOM	3221	NE2	HIS	A	417	40.502	78.656	39.122	1.00	56.98
ATOM	3222	C	HIS	A	417	36.142	77.831	39.793	1.00	67.25
ATOM	3223	O	HIS	A	417	36.302	79.055	39.738	1.00	63.87
ATOM	3224	N	LEU	A	418	35.461	77.140	38.879	1.00	68.40
ATOM	3225	CA	LEU	A	418	34.833	77.800	37.741	1.00	70.38
ATOM	3226	CB	LEU	A	418	34.168	76.781	36.810	1.00	70.71
ATOM	3227	CG	LEU	A	418	35.070	75.938	35.901	1.00	69.82
ATOM	3228	CD1	LEU	A	418	36.097	76.818	35.206	1.00	70.45
ATOM	3229	CD2	LEU	A	418	35.775	74.906	36.720	1.00	72.03
ATOM	3230	C	LEU	A	418	33.801	78.830	38.183	1.00	72.28
ATOM	3231	O	LEU	A	418	33.486	79.758	37.437	1.00	73.24
ATOM	3232	N	LYS	A	419	33.267	78.674	39.388	1.00	73.21
ATOM	3233	CA	LYS	A	419	32.293	79.636	39.881	1.00	75.47
ATOM	3234	CB	LYS	A	419	31.490	79.057	41.046	1.00	76.15
ATOM	3235	CG	LYS	A	419	30.549	77.918	40.665	1.00	78.15
ATOM	3236	CD	LYS	A	419	29.620	77.566	41.827	1.00	79.68
ATOM	3237	CE	LYS	A	419	30.404	77.229	43.096	1.00	79.88
ATOM	3238	NZ	LYS	A	419	29.516	76.965	44.262	1.00	80.23
ATOM	3239	C	LYS	A	419	32.996	80.913	40.334	1.00	76.84
ATOM	3240	O	LYS	A	419	32.739	81.993	39.806	1.00	78.50
ATOM	3241	N	SER	A	420	33.887	80.785	41.311	1.00	77.75
ATOM	3242	CA	SER	A	420	34.625	81.931	41.837	1.00	78.77
ATOM	3243	CB	SER	A	420	35.693	81.448	42.813	1.00	79.49
ATOM	3244	OG	SER	A	420	36.518	82.519	43.232	1.00	81.69

159/396

Figure 2A-59

ATOM	3245	C	SER	A	420	35.289	82.767	40.745	1.00	78.88
ATOM	3246	O	SER	A	420	35.671	83.916	40.966	1.00	79.33
ATOM	3247	N	ILE	A	421	35.429	82.170	39.570	1.00	79.17
ATOM	3248	CA	ILE	A	421	36.055	82.817	38.429	1.00	78.88
ATOM	3249	CB	ILE	A	421	36.910	81.769	37.647	1.00	79.19
ATOM	3250	CG2	ILE	A	421	36.661	81.860	36.155	1.00	80.80
ATOM	3251	CG1	ILE	A	421	38.391	81.970	37.969	1.00	79.51
ATOM	3252	CD1	ILE	A	421	38.718	81.932	39.449	1.00	79.38
ATOM	3253	C	ILE	A	421	34.992	83.462	37.528	1.00	79.44
ATOM	3254	O	ILE	A	421	35.309	84.269	36.650	1.00	78.47
ATOM	3255	N	GLY	A	422	33.731	83.108	37.758	1.00	78.35
ATOM	3256	CA	GLY	A	422	32.650	83.673	36.971	1.00	77.85
ATOM	3257	C	GLY	A	422	32.442	83.018	35.620	1.00	78.46
ATOM	3258	O	GLY	A	422	31.758	83.566	34.761	1.00	78.06
ATOM	3259	N	LEU	A	423	33.032	81.847	35.417	1.00	78.97
ATOM	3260	CA	LEU	A	423	32.869	81.149	34.154	1.00	79.57
ATOM	3261	CB	LEU	A	423	34.173	80.474	33.751	1.00	78.63
ATOM	3262	CG	LEU	A	423	35.190	81.451	33.166	1.00	79.14
ATOM	3263	CD1	LEU	A	423	36.399	80.690	32.649	1.00	77.99
ATOM	3264	CD2	LEU	A	423	34.535	82.238	32.037	1.00	79.54
ATOM	3265	C	LEU	A	423	31.739	80.134	34.233	1.00	80.65
ATOM	3266	O	LEU	A	423	31.285	79.612	33.218	1.00	81.02
ATOM	3267	N	LEU	A	424	31.294	79.860	35.451	1.00	81.93
ATOM	3268	CA	LEU	A	424	30.194	78.941	35.685	1.00	83.65
ATOM	3269	CB	LEU	A	424	30.703	77.608	36.233	1.00	83.05
ATOM	3270	CG	LEU	A	424	29.657	76.511	36.455	1.00	82.68
ATOM	3271	CD1	LEU	A	424	29.032	76.111	35.132	1.00	80.67
ATOM	3272	CD2	LEU	A	424	30.319	75.310	37.104	1.00	84.19
ATOM	3273	C	LEU	A	424	29.313	79.635	36.715	1.00	85.22
ATOM	3274	O	LEU	A	424	29.788	80.039	37.779	1.00	83.86
ATOM	3275	N	SER	A	425	28.037	79.794	36.388	1.00	87.26
ATOM	3276	CA	SER	A	425	27.105	80.462	37.287	1.00	89.33
ATOM	3277	CB	SER	A	425	25.814	80.806	36.553	1.00	89.30
ATOM	3278	OG	SER	A	425	25.132	79.623	36.182	1.00	89.97
ATOM	3279	C	SER	A	425	26.765	79.583	38.474	1.00	90.91
ATOM	3280	O	SER	A	425	26.935	78.364	38.427	1.00	91.35
ATOM	3281	N	PRO	A	426	26.288	80.197	39.564	1.00	92.68
ATOM	3282	CD	PRO	A	426	26.228	81.648	39.820	1.00	92.96
ATOM	3283	CA	PRO	A	426	25.920	79.437	40.760	1.00	94.62
ATOM	3284	CB	PRO	A	426	25.850	80.514	41.841	1.00	94.34
ATOM	3285	CG	PRO	A	426	25.388	81.719	41.077	1.00	93.81
ATOM	3286	C	PRO	A	426	24.577	78.743	40.532	1.00	96.03
ATOM	3287	O	PRO	A	426	23.946	78.252	41.471	1.00	96.20
ATOM	3288	N	ASP	A	427	24.156	78.710	39.269	1.00	98.25
ATOM	3289	CA	ASP	A	427	22.891	78.094	38.872	1.00	99.57
ATOM	3290	CB	ASP	A	427	22.253	78.900	37.731	1.00	102.12
ATOM	3291	CG	ASP	A	427	20.810	78.486	37.446	1.00	105.17
ATOM	3292	OD1	ASP	A	427	20.209	79.032	36.492	1.00	105.60
ATOM	3293	OD2	ASP	A	427	20.274	77.623	38.176	1.00	106.87
ATOM	3294	C	ASP	A	427	23.104	76.644	38.429	1.00	99.39
ATOM	3295	O	ASP	A	427	22.154	75.860	38.360	1.00	98.77
ATOM	3296	N	PHE	A	428	24.350	76.287	38.124	1.00	98.27
ATOM	3297	CA	PHE	A	428	24.646	74.925	37.701	1.00	97.61
ATOM	3298	CB	PHE	A	428	25.939	74.880	36.883	1.00	96.31
ATOM	3299	CG	PHE	A	428	26.226	73.531	36.286	1.00	94.77
ATOM	3300	CD1	PHE	A	428	26.700	72.488	37.080	1.00	94.07

160/396

Figure 2A-60

ATOM	3301	CD2	PHE	A	428	25.981	73.289	34.935	1.00	93.74
ATOM	3302	CE1	PHE	A	428	26.924	71.223	36.535	1.00	94.22
ATOM	3303	CE2	PHE	A	428	26.200	72.029	34.381	1.00	92.53
ATOM	3304	CZ	PHE	A	428	26.672	70.993	35.181	1.00	93.40
ATOM	3305	C	PHE	A	428	24.775	74.033	38.929	1.00	97.71
ATOM	3306	O	PHE	A	428	25.798	74.051	39.618	1.00	99.36
ATOM	3307	N	GLN	A	429	23.736	73.249	39.199	1.00	96.68
ATOM	3308	CA	GLN	A	429	23.743	72.369	40.357	1.00	95.14
ATOM	3309	CB	GLN	A	429	22.309	72.067	40.815	1.00	97.79
ATOM	3310	CG	GLN	A	429	21.526	71.092	39.938	1.00	99.80
ATOM	3311	CD	GLN	A	429	20.118	70.838	40.471	1.00	102.21
ATOM	3312	OE1	GLN	A	429	19.385	69.987	39.955	1.00	102.98
ATOM	3313	NE2	GLN	A	429	19.734	71.581	41.508	1.00	102.14
ATOM	3314	C	GLN	A	429	24.489	71.069	40.091	1.00	92.75
ATOM	3315	O	GLN	A	429	24.380	70.472	39.021	1.00	91.61
ATOM	3316	N	GLU	A	430	25.248	70.642	41.090	1.00	89.74
ATOM	3317	CA	GLU	A	430	26.026	69.423	41.003	1.00	86.94
ATOM	3318	CB	GLU	A	430	27.342	69.626	41.753	1.00	87.75
ATOM	3319	CG	GLU	A	430	28.008	70.963	41.434	1.00	87.29
ATOM	3320	CD	GLU	A	430	28.985	71.417	42.513	1.00	88.71
ATOM	3321	OE1	GLU	A	430	29.488	72.555	42.412	1.00	86.72
ATOM	3322	OE2	GLU	A	430	29.248	70.643	43.462	1.00	90.55
ATOM	3323	C	GLU	A	430	25.215	68.290	41.629	1.00	85.10
ATOM	3324	O	GLU	A	430	24.709	68.426	42.739	1.00	83.94
ATOM	3325	N	ASP	A	431	25.085	67.181	40.906	1.00	83.52
ATOM	3326	CA	ASP	A	431	24.331	66.025	41.390	1.00	82.44
ATOM	3327	CB	ASP	A	431	23.394	65.486	40.299	1.00	84.33
ATOM	3328	CG	ASP	A	431	22.535	66.563	39.673	1.00	87.94
ATOM	3329	OD1	ASP	A	431	21.744	67.196	40.402	1.00	91.44
ATOM	3330	OD2	ASP	A	431	22.648	66.774	38.446	1.00	90.11
ATOM	3331	C	ASP	A	431	25.284	64.901	41.773	1.00	79.90
ATOM	3332	O	ASP	A	431	26.478	64.959	41.491	1.00	80.22
ATOM	3333	N	ASN	A	432	24.751	63.870	42.415	1.00	76.52
ATOM	3334	CA	ASN	A	432	25.573	62.731	42.764	1.00	74.04
ATOM	3335	CB	ASN	A	432	24.840	61.820	43.773	1.00	74.12
ATOM	3336	CG	ASN	A	432	23.510	61.282	43.252	1.00	74.31
ATOM	3337	OD1	ASN	A	432	22.816	61.934	42.471	1.00	76.14
ATOM	3338	ND2	ASN	A	432	23.140	60.093	43.711	1.00	74.86
ATOM	3339	C	ASN	A	432	25.853	62.018	41.434	1.00	72.55
ATOM	3340	O	ASN	A	432	26.756	61.184	41.332	1.00	71.38
ATOM	3341	N	GLU	A	433	25.092	62.398	40.407	1.00	68.23
ATOM	3342	CA	GLU	A	433	25.226	61.822	39.074	1.00	66.58
ATOM	3343	CB	GLU	A	433	23.856	61.766	38.393	1.00	66.19
ATOM	3344	CG	GLU	A	433	23.069	60.522	38.742	1.00	67.41
ATOM	3345	CD	GLU	A	433	21.612	60.619	38.354	1.00	70.04
ATOM	3346	OE1	GLU	A	433	21.319	61.113	37.245	1.00	70.99
ATOM	3347	OE2	GLU	A	433	20.756	60.188	39.161	1.00	72.05
ATOM	3348	C	GLU	A	433	26.226	62.548	38.176	1.00	65.16
ATOM	3349	O	GLU	A	433	26.921	61.915	37.382	1.00	63.25
ATOM	3350	N	THR	A	434	26.282	63.872	38.284	1.00	64.12
ATOM	3351	CA	THR	A	434	27.226	64.651	37.497	1.00	64.08
ATOM	3352	CB	THR	A	434	26.933	66.161	37.589	1.00	67.81
ATOM	3353	OG1	THR	A	434	26.844	66.552	38.971	1.00	67.16
ATOM	3354	CG2	THR	A	434	25.624	66.496	36.861	1.00	66.44
ATOM	3355	C	THR	A	434	28.608	64.374	38.071	1.00	62.76
ATOM	3356	O	THR	A	434	29.618	64.602	37.422	1.00	63.26

161/396

Figure 2A-61

ATOM	3357	N	GLU	A	435	28.624	63.866	39.299	1.00	62.50
ATOM	3358	CA	GLU	A	435	29.848	63.516	40.009	1.00	62.65
ATOM	3359	CB	GLU	A	435	29.558	63.374	41.507	1.00	64.69
ATOM	3360	CG	GLU	A	435	30.485	64.142	42.435	1.00	71.10
ATOM	3361	CD	GLU	A	435	30.178	65.635	42.495	1.00	73.52
ATOM	3362	OE1	GLU	A	435	30.426	66.351	41.498	1.00	77.83
ATOM	3363	OE2	GLU	A	435	29.686	66.098	43.546	1.00	74.78
ATOM	3364	C	GLU	A	435	30.384	62.181	39.475	1.00	61.03
ATOM	3365	O	GLU	A	435	31.529	62.091	39.033	1.00	61.37
ATOM	3366	N	ILE	A	436	29.553	61.144	39.521	1.00	58.20
ATOM	3367	CA	ILE	A	436	29.965	59.836	39.040	1.00	56.35
ATOM	3368	CB	ILE	A	436	28.848	58.783	39.267	1.00	58.44
ATOM	3369	CG2	ILE	A	436	28.686	57.894	38.047	1.00	58.20
ATOM	3370	CG1	ILE	A	436	29.215	57.895	40.460	1.00	61.51
ATOM	3371	CD1	ILE	A	436	29.473	58.636	41.737	1.00	56.17
ATOM	3372	C	ILE	A	436	30.350	59.915	37.566	1.00	56.04
ATOM	3373	O	ILE	A	436	31.272	59.222	37.129	1.00	56.19
ATOM	3374	N	ASN	A	437	29.654	60.771	36.815	1.00	51.69
ATOM	3375	CA	ASN	A	437	29.932	60.975	35.396	1.00	49.69
ATOM	3376	CB	ASN	A	437	28.944	61.982	34.801	1.00	49.73
ATOM	3377	CG	ASN	A	437	27.795	61.324	34.072	1.00	53.11
ATOM	3378	OD1	ASN	A	437	27.576	60.108	34.173	1.00	51.02
ATOM	3379	ND2	ASN	A	437	27.036	62.131	33.338	1.00	48.38
ATOM	3380	C	ASN	A	437	31.339	61.537	35.217	1.00	50.55
ATOM	3381	O	ASN	A	437	32.039	61.226	34.242	1.00	50.39
ATOM	3382	N	PHE	A	438	31.739	62.393	36.152	1.00	47.85
ATOM	3383	CA	PHE	A	438	33.050	63.018	36.091	1.00	47.43
ATOM	3384	CB	PHE	A	438	33.075	64.263	36.990	1.00	46.14
ATOM	3385	CG	PHE	A	438	34.437	64.882	37.121	1.00	47.69
ATOM	3386	CD1	PHE	A	438	35.039	65.505	36.032	1.00	48.11
ATOM	3387	CD2	PHE	A	438	35.142	64.787	38.314	1.00	47.23
ATOM	3388	CE1	PHE	A	438	36.333	66.022	36.123	1.00	47.20
ATOM	3389	CE2	PHE	A	438	36.430	65.299	38.419	1.00	49.80
ATOM	3390	CZ	PHE	A	438	37.029	65.916	37.322	1.00	50.20
ATOM	3391	C	PHE	A	438	34.151	62.039	36.512	1.00	45.39
ATOM	3392	O	PHE	A	438	35.200	61.963	35.881	1.00	45.23
ATOM	3393	N	LEU	A	439	33.896	61.303	37.587	1.00	45.36
ATOM	3394	CA	LEU	A	439	34.836	60.327	38.119	1.00	45.53
ATOM	3395	CB	LEU	A	439	34.326	59.833	39.484	1.00	46.26
ATOM	3396	CG	LEU	A	439	35.041	60.285	40.772	1.00	49.23
ATOM	3397	CD1	LEU	A	439	35.681	61.639	40.571	1.00	45.88
ATOM	3398	CD2	LEU	A	439	34.060	60.304	41.948	1.00	42.94
ATOM	3399	C	LEU	A	439	35.054	59.148	37.156	1.00	44.39
ATOM	3400	O	LEU	A	439	36.167	58.638	37.028	1.00	44.71
ATOM	3401	N	LEU	A	440	33.988	58.723	36.482	1.00	44.54
ATOM	3402	CA	LEU	A	440	34.073	57.621	35.531	1.00	42.64
ATOM	3403	CB	LEU	A	440	32.661	57.222	35.040	1.00	43.07
ATOM	3404	CG	LEU	A	440	32.444	56.133	33.968	1.00	41.02
ATOM	3405	CD1	LEU	A	440	32.861	56.657	32.584	1.00	39.71
ATOM	3406	CD2	LEU	A	440	33.238	54.891	34.324	1.00	39.94
ATOM	3407	C	LEU	A	440	34.922	58.121	34.378	1.00	41.96
ATOM	3408	O	LEU	A	440	35.825	57.427	33.914	1.00	42.69
ATOM	3409	N	LYS	A	441	34.651	59.340	33.923	1.00	41.67
ATOM	3410	CA	LYS	A	441	35.438	59.888	32.822	1.00	43.70
ATOM	3411	CB	LYS	A	441	34.923	61.277	32.426	1.00	44.75
ATOM	3412	CG	LYS	A	441	35.698	61.888	31.256	1.00	48.41

162/396

Figure 2A-62

ATOM	3413	CD	LYS	A	441	35.147	63.244	30.839	1.00	53.00
ATOM	3414	CE	LYS	A	441	36.021	63.853	29.749	1.00	59.86
ATOM	3415	NZ	LYS	A	441	36.340	62.855	28.676	1.00	65.01
ATOM	3416	C	LYS	A	441	36.923	59.973	33.217	1.00	42.97
ATOM	3417	O	LYS	A	441	37.810	59.693	32.415	1.00	40.15
ATOM	3418	N	GLN	A	442	37.181	60.373	34.456	1.00	42.07
ATOM	3419	CA	GLN	A	442	38.550	60.481	34.967	1.00	41.42
ATOM	3420	CB	GLN	A	442	38.525	61.085	36.370	1.00	43.41
ATOM	3421	CG	GLN	A	442	38.217	62.548	36.386	1.00	41.12
ATOM	3422	CD	GLN	A	442	39.381	63.342	35.884	1.00	43.68
ATOM	3423	OE1	GLN	A	442	40.189	63.850	36.672	1.00	48.28
ATOM	3424	NE2	GLN	A	442	39.500	63.444	34.568	1.00	46.15
ATOM	3425	C	GLN	A	442	39.220	59.114	35.036	1.00	39.32
ATOM	3426	O	GLN	A	442	40.380	58.962	34.665	1.00	38.04
ATOM	3427	N	ALA	A	443	38.470	58.125	35.515	1.00	37.83
ATOM	3428	CA	ALA	A	443	38.981	56.767	35.677	1.00	37.23
ATOM	3429	CB	ALA	A	443	37.967	55.947	36.467	1.00	34.21
ATOM	3430	C	ALA	A	443	39.330	56.071	34.346	1.00	38.26
ATOM	3431	O	ALA	A	443	40.301	55.296	34.278	1.00	31.79
ATOM	3432	N	LEU	A	444	38.554	56.359	33.294	1.00	38.69
ATOM	3433	CA	LEU	A	444	38.797	55.766	31.972	1.00	42.14
ATOM	3434	CB	LEU	A	444	37.773	56.282	30.958	1.00	40.96
ATOM	3435	CG	LEU	A	444	36.585	55.435	30.495	1.00	44.07
ATOM	3436	CD1	LEU	A	444	36.361	54.222	31.351	1.00	40.60
ATOM	3437	CD2	LEU	A	444	35.374	56.340	30.445	1.00	40.44
ATOM	3438	C	LEU	A	444	40.196	56.115	31.479	1.00	44.10
ATOM	3439	O	LEU	A	444	40.847	55.325	30.779	1.00	43.48
ATOM	3440	N	THR	A	445	40.646	57.319	31.819	1.00	44.74
ATOM	3441	CA	THR	A	445	41.979	57.776	31.433	1.00	45.47
ATOM	3442	CB	THR	A	445	42.002	59.302	31.267	1.00	47.77
ATOM	3443	OG1	THR	A	445	41.014	59.678	30.303	1.00	53.61
ATOM	3444	CG2	THR	A	445	43.370	59.784	30.798	1.00	41.04
ATOM	3445	C	THR	A	445	43.023	57.401	32.498	1.00	45.55
ATOM	3446	O	THR	A	445	44.012	56.713	32.218	1.00	44.89
ATOM	3447	N	ILE	A	446	42.779	57.853	33.724	1.00	46.90
ATOM	3448	CA	ILE	A	446	43.699	57.620	34.837	1.00	46.76
ATOM	3449	CB	ILE	A	446	43.337	58.535	36.015	1.00	44.77
ATOM	3450	CG2	ILE	A	446	44.150	58.151	37.240	1.00	46.43
ATOM	3451	CG1	ILE	A	446	43.608	59.989	35.618	1.00	42.66
ATOM	3452	CD1	ILE	A	446	42.660	60.980	36.244	1.00	37.66
ATOM	3453	C	ILE	A	446	43.842	56.180	35.328	1.00	44.29
ATOM	3454	O	ILE	A	446	44.953	55.662	35.365	1.00	45.97
ATOM	3455	N	VAL	A	447	42.742	55.533	35.704	1.00	43.25
ATOM	3456	CA	VAL	A	447	42.819	54.151	36.169	1.00	43.46
ATOM	3457	CB	VAL	A	447	41.547	53.751	36.963	1.00	43.74
ATOM	3458	CG1	VAL	A	447	41.624	52.281	37.378	1.00	42.47
ATOM	3459	CG2	VAL	A	447	41.413	54.630	38.213	1.00	42.88
ATOM	3460	C	VAL	A	447	43.038	53.152	35.020	1.00	45.22
ATOM	3461	O	VAL	A	447	43.859	52.243	35.132	1.00	47.41
ATOM	3462	N	GLY	A	448	42.318	53.322	33.912	1.00	45.43
ATOM	3463	CA	GLY	A	448	42.466	52.405	32.793	1.00	39.39
ATOM	3464	C	GLY	A	448	43.890	52.221	32.286	1.00	40.49
ATOM	3465	O	GLY	A	448	44.267	51.141	31.840	1.00	40.82
ATOM	3466	N	THR	A	449	44.700	53.270	32.375	1.00	39.02
ATOM	3467	CA	THR	A	449	46.076	53.214	31.903	1.00	33.05
ATOM	3468	CB	THR	A	449	46.576	54.638	31.549	1.00	36.37

163/396

Figure 2A-63

ATOM	3469	OG1	THR	A	449	47.692	54.541	30.660	1.00	37.51
ATOM	3470	CG2	THR	A	449	47.023	55.392	32.821	1.00	32.28
ATOM	3471	C	THR	A	449	47.086	52.587	32.878	1.00	35.13
ATOM	3472	O	THR	A	449	48.182	52.190	32.468	1.00	36.17
ATOM	3473	N	LEU	A	450	46.745	52.499	34.157	1.00	34.38
ATOM	3474	CA	LEU	A	450	47.694	51.934	35.119	1.00	38.26
ATOM	3475	CB	LEU	A	450	47.169	52.097	36.548	1.00	33.30
ATOM	3476	CG	LEU	A	450	47.271	53.563	36.971	1.00	37.58
ATOM	3477	CD1	LEU	A	450	46.687	53.758	38.365	1.00	39.70
ATOM	3478	CD2	LEU	A	450	48.740	53.989	36.921	1.00	33.90
ATOM	3479	C	LEU	A	450	48.068	50.480	34.843	1.00	36.83
ATOM	3480	O	LEU	A	450	49.240	50.142	34.779	1.00	38.36
ATOM	3481	N	PRO	A	451	47.078	49.607	34.643	1.00	38.71
ATOM	3482	CD	PRO	A	451	45.616	49.733	34.745	1.00	40.57
ATOM	3483	CA	PRO	A	451	47.448	48.222	34.379	1.00	36.82
ATOM	3484	CB	PRO	A	451	46.093	47.506	34.368	1.00	38.03
ATOM	3485	CG	PRO	A	451	45.243	48.360	35.243	1.00	38.71
ATOM	3486	C	PRO	A	451	48.183	48.107	33.055	1.00	36.27
ATOM	3487	O	PRO	A	451	49.103	47.299	32.919	1.00	37.84
ATOM	3488	N	PHE	A	452	47.783	48.924	32.078	1.00	36.91
ATOM	3489	CA	PHE	A	452	48.416	48.896	30.761	1.00	36.11
ATOM	3490	CB	PHE	A	452	47.652	49.814	29.776	1.00	38.23
ATOM	3491	CG	PHE	A	452	48.353	50.004	28.452	1.00	38.59
ATOM	3492	CD1	PHE	A	452	49.488	50.822	28.356	1.00	37.37
ATOM	3493	CD2	PHE	A	452	47.913	49.329	27.315	1.00	41.10
ATOM	3494	CE1	PHE	A	452	50.175	50.959	27.159	1.00	39.36
ATOM	3495	CE2	PHE	A	452	48.592	49.457	26.097	1.00	42.11
ATOM	3496	CZ	PHE	A	452	49.731	50.276	26.020	1.00	42.26
ATOM	3497	C	PHE	A	452	49.873	49.322	30.867	1.00	36.09
ATOM	3498	O	PHE	A	452	50.760	48.706	30.281	1.00	33.77
ATOM	3499	N	THR	A	453	50.120	50.372	31.644	1.00	39.02
ATOM	3500	CA	THR	A	453	51.470	50.888	31.827	1.00	38.00
ATOM	3501	CB	THR	A	453	51.424	52.241	32.558	1.00	41.95
ATOM	3502	OG1	THR	A	453	50.611	53.134	31.796	1.00	36.38
ATOM	3503	CG2	THR	A	453	52.846	52.817	32.759	1.00	35.46
ATOM	3504	C	THR	A	453	52.361	49.923	32.600	1.00	36.80
ATOM	3505	O	THR	A	453	53.485	49.642	32.177	1.00	36.83
ATOM	3506	N	TYR	A	454	51.874	49.414	33.725	1.00	37.93
ATOM	3507	CA	TYR	A	454	52.676	48.461	34.504	1.00	40.63
ATOM	3508	CB	TYR	A	454	51.924	48.027	35.769	1.00	40.89
ATOM	3509	CG	TYR	A	454	52.481	46.763	36.397	1.00	46.23
ATOM	3510	CD1	TYR	A	454	51.671	45.652	36.600	1.00	49.38
ATOM	3511	CE1	TYR	A	454	52.185	44.464	37.132	1.00	54.67
ATOM	3512	CD2	TYR	A	454	53.829	46.667	36.748	1.00	51.05
ATOM	3513	CE2	TYR	A	454	54.359	45.489	37.286	1.00	53.88
ATOM	3514	CZ	TYR	A	454	53.528	44.389	37.473	1.00	54.62
ATOM	3515	OH	TYR	A	454	54.038	43.220	37.989	1.00	56.04
ATOM	3516	C	TYR	A	454	53.003	47.225	33.661	1.00	39.78
ATOM	3517	O	TYR	A	454	54.137	46.786	33.582	1.00	41.84
ATOM	3518	N	MET	A	455	51.998	46.663	33.012	1.00	44.50
ATOM	3519	CA	MET	A	455	52.225	45.473	32.214	1.00	45.08
ATOM	3520	CB	MET	A	455	50.894	44.967	31.659	1.00	46.34
ATOM	3521	CG	MET	A	455	50.989	43.679	30.881	1.00	50.91
ATOM	3522	SD	MET	A	455	51.115	43.962	29.117	1.00	50.30
ATOM	3523	CE	MET	A	455	52.620	43.128	28.722	1.00	50.86
ATOM	3524	C	MET	A	455	53.243	45.694	31.100	1.00	45.04

164/396

Figure 2A-64

ATOM	3525	O	MET	A	455	54.144	44.879	30.908	1.00	43.92
ATOM	3526	N	LEU	A	456	53.130	46.800	30.371	1.00	45.37
ATOM	3527	CA	LEU	A	456	54.092	47.055	29.301	1.00	41.86
ATOM	3528	CB	LEU	A	456	53.686	48.331	28.533	1.00	40.84
ATOM	3529	CG	LEU	A	456	54.557	49.283	27.679	1.00	41.23
ATOM	3530	CD1	LEU	A	456	55.941	48.774	27.495	1.00	39.22
ATOM	3531	CD2	LEU	A	456	53.867	49.527	26.309	1.00	39.76
ATOM	3532	C	LEU	A	456	55.528	47.126	29.850	1.00	39.35
ATOM	3533	O	LEU	A	456	56.418	46.451	29.343	1.00	40.17
ATOM	3534	N	GLU	A	457	55.773	47.926	30.875	1.00	41.68
ATOM	3535	CA	GLU	A	457	57.136	48.007	31.420	1.00	44.16
ATOM	3536	CB	GLU	A	457	57.228	49.107	32.471	1.00	44.34
ATOM	3537	CG	GLU	A	457	57.507	50.482	31.894	1.00	53.00
ATOM	3538	CD	GLU	A	457	58.923	50.638	31.328	1.00	48.33
ATOM	3539	OE1	GLU	A	457	59.660	51.510	31.826	1.00	46.33
ATOM	3540	OE2	GLU	A	457	59.292	49.907	30.386	1.00	49.74
ATOM	3541	C	GLU	A	457	57.647	46.690	32.023	1.00	43.08
ATOM	3542	O	GLU	A	457	58.852	46.394	31.978	1.00	41.95
ATOM	3543	N	LYS	A	458	56.736	45.907	32.590	1.00	44.89
ATOM	3544	CA	LYS	A	458	57.113	44.629	33.181	1.00	46.87
ATOM	3545	CB	LYS	A	458	55.908	43.975	33.847	1.00	51.86
ATOM	3546	CG	LYS	A	458	56.204	42.605	34.447	1.00	57.79
ATOM	3547	CD	LYS	A	458	57.196	42.693	35.604	1.00	59.75
ATOM	3548	CE	LYS	A	458	57.300	41.351	36.352	1.00	62.74
ATOM	3549	NZ	LYS	A	458	58.322	41.375	37.440	1.00	60.49
ATOM	3550	C	LYS	A	458	57.640	43.730	32.078	1.00	47.43
ATOM	3551	O	LYS	A	458	58.685	43.079	32.234	1.00	47.56
ATOM	3552	N	TRP	A	459	56.938	43.714	30.945	1.00	43.67
ATOM	3553	CA	TRP	A	459	57.370	42.903	29.830	1.00	43.34
ATOM	3554	CB	TRP	A	459	56.384	43.019	28.678	1.00	44.39
ATOM	3555	CG	TRP	A	459	56.731	42.158	27.502	1.00	39.17
ATOM	3556	CD2	TRP	A	459	57.507	42.538	26.364	1.00	38.74
ATOM	3557	CE2	TRP	A	459	57.537	41.426	25.488	1.00	37.33
ATOM	3558	CE3	TRP	A	459	58.180	43.711	25.996	1.00	38.95
ATOM	3559	CD1	TRP	A	459	56.340	40.866	27.285	1.00	41.15
ATOM	3560	NE1	TRP	A	459	56.819	40.420	26.076	1.00	40.20
ATOM	3561	CZ2	TRP	A	459	58.210	41.452	24.269	1.00	39.01
ATOM	3562	CZ3	TRP	A	459	58.852	43.746	24.784	1.00	36.17
ATOM	3563	CH2	TRP	A	459	58.862	42.620	23.929	1.00	44.08
ATOM	3564	C	TRP	A	459	58.768	43.326	29.379	1.00	45.95
ATOM	3565	O	TRP	A	459	59.628	42.477	29.127	1.00	46.98
ATOM	3566	N	ARG	A	460	59.010	44.632	29.288	1.00	45.80
ATOM	3567	CA	ARG	A	460	60.331	45.115	28.871	1.00	45.86
ATOM	3568	CB	ARG	A	460	60.341	46.627	28.685	1.00	48.11
ATOM	3569	CG	ARG	A	460	59.628	47.152	27.463	1.00	51.85
ATOM	3570	CD	ARG	A	460	59.327	48.610	27.744	1.00	50.43
ATOM	3571	NE	ARG	A	460	59.969	49.482	26.796	1.00	44.58
ATOM	3572	CZ	ARG	A	460	59.942	50.805	26.867	1.00	41.47
ATOM	3573	NH1	ARG	A	460	59.317	51.414	27.867	1.00	35.56
ATOM	3574	NH2	ARG	A	460	60.478	51.515	25.882	1.00	38.64
ATOM	3575	C	ARG	A	460	61.403	44.778	29.900	1.00	43.01
ATOM	3576	O	ARG	A	460	62.506	44.378	29.543	1.00	41.66
ATOM	3577	N	TRP	A	461	61.092	44.995	31.173	1.00	41.97
ATOM	3578	CA	TRP	A	461	62.046	44.681	32.236	1.00	43.93
ATOM	3579	CB	TRP	A	461	61.416	44.916	33.613	1.00	39.98
ATOM	3580	CG	TRP	A	461	61.320	46.372	33.969	1.00	38.05

165/396

Figure 2A-65

ATOM	3581	CD2	TRP	A	461	60.506	46.950	34.991	1.00	35.56
ATOM	3582	CE2	TRP	A	461	60.799	48.329	35.027	1.00	36.95
ATOM	3583	CE3	TRP	A	461	59.557	46.436	35.883	1.00	41.04
ATOM	3584	CD1	TRP	A	461	62.050	47.398	33.431	1.00	34.58
ATOM	3585	NE1	TRP	A	461	61.745	48.575	34.064	1.00	36.66
ATOM	3586	CZ2	TRP	A	461	60.178	49.201	35.920	1.00	34.86
ATOM	3587	CZ3	TRP	A	461	58.935	47.301	36.772	1.00	41.28
ATOM	3588	CH2	TRP	A	461	59.251	48.674	36.782	1.00	39.21
ATOM	3589	C	TRP	A	461	62.488	43.227	32.125	1.00	43.24
ATOM	3590	O	TRP	A	461	63.680	42.918	32.202	1.00	43.65
ATOM	3591	N	MET	A	462	61.513	42.347	31.913	1.00	46.02
ATOM	3592	CA	MET	A	462	61.775	40.922	31.797	1.00	48.60
ATOM	3593	CB	MET	A	462	60.465	40.145	31.839	1.00	49.33
ATOM	3594	CG	MET	A	462	59.771	40.212	33.190	1.00	47.35
ATOM	3595	SD	MET	A	462	58.189	39.343	33.127	1.00	54.41
ATOM	3596	CE	MET	A	462	58.685	37.717	33.770	1.00	52.65
ATOM	3597	C	MET	A	462	62.552	40.574	30.541	1.00	50.74
ATOM	3598	O	MET	A	462	63.429	39.694	30.565	1.00	50.35
ATOM	3599	N	VAL	A	463	62.232	41.261	29.447	1.00	50.83
ATOM	3600	CA	VAL	A	463	62.927	41.044	28.190	1.00	46.55
ATOM	3601	CB	VAL	A	463	62.319	41.901	27.052	1.00	46.34
ATOM	3602	CG1	VAL	A	463	63.278	41.969	25.880	1.00	41.87
ATOM	3603	CG2	VAL	A	463	60.989	41.294	26.594	1.00	47.30
ATOM	3604	C	VAL	A	463	64.391	41.433	28.381	1.00	50.88
ATOM	3605	O	VAL	A	463	65.289	40.678	28.014	1.00	50.37
ATOM	3606	N	PHE	A	464	64.638	42.604	28.964	1.00	51.26
ATOM	3607	CA	PHE	A	464	66.017	43.061	29.171	1.00	55.78
ATOM	3608	CB	PHE	A	464	66.032	44.505	29.706	1.00	55.50
ATOM	3609	CG	PHE	A	464	65.486	45.521	28.734	1.00	57.79
ATOM	3610	CD1	PHE	A	464	64.666	46.552	29.171	1.00	58.46
ATOM	3611	CD2	PHE	A	464	65.776	45.436	27.381	1.00	61.28
ATOM	3612	CE1	PHE	A	464	64.146	47.476	28.272	1.00	60.09
ATOM	3613	CE2	PHE	A	464	65.260	46.358	26.475	1.00	61.16
ATOM	3614	CZ	PHE	A	464	64.446	47.375	26.922	1.00	60.32
ATOM	3615	C	PHE	A	464	66.804	42.134	30.117	1.00	56.75
ATOM	3616	O	PHE	A	464	68.023	41.970	29.968	1.00	56.31
ATOM	3617	N	LYS	A	465	66.110	41.538	31.085	1.00	56.63
ATOM	3618	CA	LYS	A	465	66.757	40.615	32.019	1.00	56.24
ATOM	3619	CB	LYS	A	465	65.882	40.389	33.248	1.00	52.98
ATOM	3620	CG	LYS	A	465	65.840	41.558	34.187	1.00	54.76
ATOM	3621	CD	LYS	A	465	64.900	41.296	35.349	1.00	56.17
ATOM	3622	CE	LYS	A	465	65.064	42.382	36.399	1.00	56.74
ATOM	3623	NZ	LYS	A	465	64.220	42.162	37.598	1.00	58.89
ATOM	3624	C	LYS	A	465	67.043	39.271	31.358	1.00	54.79
ATOM	3625	O	LYS	A	465	67.866	38.509	31.835	1.00	56.57
ATOM	3626	N	GLY	A	466	66.367	38.991	30.252	1.00	55.12
ATOM	3627	CA	GLY	A	466	66.572	37.731	29.562	1.00	55.95
ATOM	3628	C	GLY	A	466	65.698	36.596	30.086	1.00	56.55
ATOM	3629	O	GLY	A	466	66.038	35.429	29.924	1.00	59.42
ATOM	3630	N	GLU	A	467	64.575	36.933	30.711	1.00	56.13
ATOM	3631	CA	GLU	A	467	63.666	35.932	31.257	1.00	56.01
ATOM	3632	CB	GLU	A	467	62.970	36.470	32.493	1.00	55.63
ATOM	3633	CG	GLU	A	467	63.900	37.130	33.469	1.00	60.08
ATOM	3634	CD	GLU	A	467	63.157	37.679	34.655	1.00	64.69
ATOM	3635	OE1	GLU	A	467	62.129	38.356	34.440	1.00	67.53
ATOM	3636	OE2	GLU	A	467	63.595	37.441	35.801	1.00	68.11

166/396

Figure 2A-66

ATOM	3637	C	GLU	A	467	62.614	35.516	30.247	1.00	57.20
ATOM	3638	O	GLU	A	467	61.820	34.617	30.512	1.00	57.04
ATOM	3639	N	ILE	A	468	62.590	36.182	29.097	1.00	57.42
ATOM	3640	CA	ILE	A	468	61.638	35.825	28.058	1.00	58.66
ATOM	3641	CB	ILE	A	468	60.559	36.902	27.848	1.00	56.02
ATOM	3642	CG2	ILE	A	468	59.558	36.406	26.821	1.00	54.28
ATOM	3643	CG1	ILE	A	468	59.837	37.215	29.158	1.00	54.32
ATOM	3644	CD1	ILE	A	468	58.935	38.443	29.067	1.00	49.25
ATOM	3645	C	ILE	A	468	62.400	35.638	26.746	1.00	61.27
ATOM	3646	O	ILE	A	468	62.746	36.603	26.068	1.00	62.63
ATOM	3647	N	PRO	A	469	62.677	34.383	26.380	1.00	62.86
ATOM	3648	CD	PRO	A	469	62.250	33.162	27.085	1.00	62.42
ATOM	3649	CA	PRO	A	469	63.401	34.056	25.147	1.00	62.34
ATOM	3650	CB	PRO	A	469	63.334	32.531	25.102	1.00	63.91
ATOM	3651	CG	PRO	A	469	63.232	32.149	26.564	1.00	65.78
ATOM	3652	C	PRO	A	469	62.718	34.679	23.937	1.00	60.80
ATOM	3653	O	PRO	A	469	61.493	34.781	23.901	1.00	60.28
ATOM	3654	N	LYS	A	470	63.510	35.085	22.950	1.00	59.91
ATOM	3655	CA	LYS	A	470	62.968	35.689	21.736	1.00	59.36
ATOM	3656	CB	LYS	A	470	64.034	35.746	20.631	1.00	59.78
ATOM	3657	CG	LYS	A	470	65.220	36.681	20.887	1.00	64.76
ATOM	3658	CD	LYS	A	470	66.242	36.588	19.741	1.00	67.09
ATOM	3659	CE	LYS	A	470	67.510	37.410	20.008	1.00	72.78
ATOM	3660	NZ	LYS	A	470	67.288	38.903	20.021	1.00	74.61
ATOM	3661	C	LYS	A	470	61.770	34.885	21.226	1.00	58.05
ATOM	3662	O	LYS	A	470	60.764	35.463	20.793	1.00	53.94
ATOM	3663	N	ASP	A	471	61.877	33.554	21.293	1.00	57.97
ATOM	3664	CA	ASP	A	471	60.805	32.678	20.809	1.00	57.27
ATOM	3665	CB	ASP	A	471	61.308	31.236	20.616	1.00	60.60
ATOM	3666	CG	ASP	A	471	61.937	30.648	21.868	1.00	64.67
ATOM	3667	OD1	ASP	A	471	61.218	30.404	22.864	1.00	64.62
ATOM	3668	OD2	ASP	A	471	63.167	30.426	21.849	1.00	69.75
ATOM	3669	C	ASP	A	471	59.531	32.676	21.634	1.00	53.93
ATOM	3670	O	ASP	A	471	58.565	32.018	21.264	1.00	53.16
ATOM	3671	N	GLN	A	472	59.521	33.423	22.738	1.00	53.28
ATOM	3672	CA	GLN	A	472	58.327	33.529	23.582	1.00	52.32
ATOM	3673	CB	GLN	A	472	58.562	32.870	24.937	1.00	54.17
ATOM	3674	CG	GLN	A	472	59.006	31.434	24.865	1.00	60.74
ATOM	3675	CD	GLN	A	472	58.521	30.657	26.063	1.00	63.97
ATOM	3676	OE1	GLN	A	472	58.861	30.974	27.210	1.00	63.75
ATOM	3677	NE2	GLN	A	472	57.702	29.639	25.808	1.00	65.08
ATOM	3678	C	GLN	A	472	57.872	34.978	23.835	1.00	48.44
ATOM	3679	O	GLN	A	472	56.972	35.209	24.647	1.00	46.89
ATOM	3680	N	TRP	A	473	58.491	35.940	23.156	1.00	46.79
ATOM	3681	CA	TRP	A	473	58.145	37.355	23.335	1.00	45.37
ATOM	3682	CB	TRP	A	473	58.899	38.224	22.335	1.00	46.66
ATOM	3683	CG	TRP	A	473	60.273	38.573	22.748	1.00	48.12
ATOM	3684	CD2	TRP	A	473	61.146	39.507	22.099	1.00	48.02
ATOM	3685	CE2	TRP	A	473	62.364	39.511	22.820	1.00	47.01
ATOM	3686	CE3	TRP	A	473	61.016	40.341	20.978	1.00	46.67
ATOM	3687	CD1	TRP	A	473	60.971	38.065	23.802	1.00	49.72
ATOM	3688	NE1	TRP	A	473	62.230	38.623	23.854	1.00	46.63
ATOM	3689	CZ2	TRP	A	473	63.448	40.317	22.457	1.00	47.85
ATOM	3690	CZ3	TRP	A	473	62.093	41.145	20.615	1.00	47.89
ATOM	3691	CH2	TRP	A	473	63.295	41.126	21.355	1.00	50.93
ATOM	3692	C	TRP	A	473	56.660	37.649	23.202	1.00	43.79

167/396

Figure 2A-67

ATOM	3693	O	TRP	A 473	56.034	38.135	24.144	1.00	42.98
ATOM	3694	N	MET	A 474	56.095	37.384	22.028	1.00	42.30
ATOM	3695	CA	MET	A 474	54.677	37.639	21.834	1.00	42.82
ATOM	3696	CB	MET	A 474	54.278	37.463	20.361	1.00	44.84
ATOM	3697	CG	MET	A 474	54.844	38.523	19.420	1.00	46.36
ATOM	3698	SD	MET	A 474	54.752	40.170	20.154	1.00	49.32
ATOM	3699	CE	MET	A 474	53.071	40.359	20.240	1.00	48.72
ATOM	3700	C	MET	A 474	53.815	36.734	22.702	1.00	45.75
ATOM	3701	O	MET	A 474	52.790	37.170	23.235	1.00	47.04
ATOM	3702	N	LYS	A 475	54.216	35.473	22.849	1.00	46.83
ATOM	3703	CA	LYS	A 475	53.434	34.562	23.666	1.00	45.76
ATOM	3704	CB	LYS	A 475	54.094	33.177	23.749	1.00	47.43
ATOM	3705	CG	LYS	A 475	53.202	32.141	24.416	1.00	48.96
ATOM	3706	CD	LYS	A 475	54.013	31.158	25.239	1.00	57.74
ATOM	3707	CE	LYS	A 475	54.082	29.778	24.589	1.00	60.64
ATOM	3708	NZ	LYS	A 475	52.761	29.067	24.629	1.00	64.20
ATOM	3709	C	LYS	A 475	53.318	35.154	25.064	1.00	44.03
ATOM	3710	O	LYS	A 475	52.222	35.265	25.615	1.00	41.76
ATOM	3711	N	LYS	A 476	54.450	35.556	25.628	1.00	43.04
ATOM	3712	CA	LYS	A 476	54.435	36.122	26.966	1.00	45.42
ATOM	3713	CB	LYS	A 476	55.862	36.274	27.495	1.00	46.83
ATOM	3714	CG	LYS	A 476	56.128	35.492	28.776	1.00	53.29
ATOM	3715	CD	LYS	A 476	55.190	35.918	29.888	1.00	59.00
ATOM	3716	CE	LYS	A 476	55.602	35.329	31.232	1.00	65.08
ATOM	3717	NZ	LYS	A 476	55.614	33.821	31.220	1.00	69.99
ATOM	3718	C	LYS	A 476	53.712	37.464	27.008	1.00	46.40
ATOM	3719	O	LYS	A 476	53.040	37.783	27.997	1.00	46.99
ATOM	3720	N	TRP	A 477	53.838	38.245	25.936	1.00	43.64
ATOM	3721	CA	TRP	A 477	53.179	39.545	25.878	1.00	43.75
ATOM	3722	CB	TRP	A 477	53.522	40.265	24.569	1.00	41.93
ATOM	3723	CG	TRP	A 477	52.726	41.525	24.298	1.00	44.61
ATOM	3724	CD2	TRP	A 477	52.988	42.838	24.811	1.00	41.16
ATOM	3725	CE2	TRP	A 477	52.041	43.717	24.220	1.00	43.88
ATOM	3726	CE3	TRP	A 477	53.930	43.361	25.709	1.00	41.79
ATOM	3727	CD1	TRP	A 477	51.657	41.655	23.449	1.00	44.96
ATOM	3728	NE1	TRP	A 477	51.246	42.966	23.394	1.00	44.58
ATOM	3729	CZ2	TRP	A 477	52.008	45.101	24.499	1.00	40.51
ATOM	3730	CZ3	TRP	A 477	53.902	44.742	25.993	1.00	44.73
ATOM	3731	CH2	TRP	A 477	52.938	45.594	25.382	1.00	42.22
ATOM	3732	C	TRP	A 477	51.677	39.377	26.000	1.00	42.36
ATOM	3733	O	TRP	A 477	51.047	40.039	26.811	1.00	47.21
ATOM	3734	N	TRP	A 478	51.098	38.488	25.200	1.00	45.68
ATOM	3735	CA	TRP	A 478	49.658	38.271	25.248	1.00	43.28
ATOM	3736	CB	TRP	A 478	49.180	37.627	23.948	1.00	44.66
ATOM	3737	CG	TRP	A 478	49.147	38.676	22.872	1.00	44.09
ATOM	3738	CD2	TRP	A 478	48.321	39.844	22.877	1.00	38.01
ATOM	3739	CE2	TRP	A 478	48.765	40.677	21.835	1.00	38.55
ATOM	3740	CE3	TRP	A 478	47.253	40.267	23.674	1.00	37.72
ATOM	3741	CD1	TRP	A 478	50.026	38.832	21.839	1.00	42.06
ATOM	3742	NE1	TRP	A 478	49.808	40.041	21.214	1.00	41.80
ATOM	3743	CZ2	TRP	A 478	48.178	41.919	21.569	1.00	38.40
ATOM	3744	CZ3	TRP	A 478	46.670	41.502	23.412	1.00	39.35
ATOM	3745	CH2	TRP	A 478	47.138	42.312	22.368	1.00	37.00
ATOM	3746	C	TRP	A 478	49.210	37.481	26.467	1.00	44.95
ATOM	3747	O	TRP	A 478	48.079	37.619	26.917	1.00	47.27
ATOM	3748	N	GLU	A 479	50.102	36.684	27.032	1.00	45.53

168/396

Figure 2A-68

ATOM	3749	CA	GLU	A	479	49.759	35.932	28.238	1.00	48.89
ATOM	3750	CB	GLU	A	479	50.901	34.973	28.591	1.00	52.23
ATOM	3751	CG	GLU	A	479	50.478	33.567	28.973	1.00	58.20
ATOM	3752	CD	GLU	A	479	51.444	32.508	28.439	1.00	62.80
ATOM	3753	OE1	GLU	A	479	52.627	32.500	28.859	1.00	62.47
ATOM	3754	OE2	GLU	A	479	51.013	31.687	27.593	1.00	64.64
ATOM	3755	C	GLU	A	479	49.604	36.991	29.333	1.00	47.36
ATOM	3756	O	GLU	A	479	48.695	36.925	30.166	1.00	47.62
ATOM	3757	N	MET	A	480	50.496	37.983	29.302	1.00	47.21
ATOM	3758	CA	MET	A	480	50.489	39.080	30.267	1.00	44.41
ATOM	3759	CB	MET	A	480	51.848	39.774	30.239	1.00	46.86
ATOM	3760	CG	MET	A	480	52.951	38.923	30.861	1.00	42.40
ATOM	3761	SD	MET	A	480	54.613	39.515	30.555	1.00	48.70
ATOM	3762	CE	MET	A	480	54.659	40.916	31.734	1.00	38.78
ATOM	3763	C	MET	A	480	49.346	40.091	30.060	1.00	45.75
ATOM	3764	O	MET	A	480	48.802	40.640	31.030	1.00	42.68
ATOM	3765	N	LYS	A	481	48.973	40.344	28.806	1.00	45.17
ATOM	3766	CA	LYS	A	481	47.858	41.256	28.552	1.00	46.38
ATOM	3767	CB	LYS	A	481	47.656	41.458	27.042	1.00	47.55
ATOM	3768	CG	LYS	A	481	48.539	42.519	26.403	1.00	51.88
ATOM	3769	CD	LYS	A	481	48.099	43.934	26.815	1.00	54.17
ATOM	3770	CE	LYS	A	481	48.725	45.003	25.922	1.00	54.40
ATOM	3771	NZ	LYS	A	481	48.167	46.366	26.211	1.00	55.74
ATOM	3772	C	LYS	A	481	46.585	40.657	29.168	1.00	47.27
ATOM	3773	O	LYS	A	481	45.817	41.357	29.839	1.00	47.89
ATOM	3774	N	ARG	A	482	46.379	39.355	28.932	1.00	48.39
ATOM	3775	CA	ARG	A	482	45.216	38.609	29.428	1.00	47.02
ATOM	3776	CB	ARG	A	482	45.226	37.169	28.894	1.00	50.92
ATOM	3777	CG	ARG	A	482	44.982	37.015	27.399	1.00	54.51
ATOM	3778	CD	ARG	A	482	45.246	35.574	26.950	1.00	56.76
ATOM	3779	NE	ARG	A	482	45.067	35.374	25.511	1.00	58.94
ATOM	3780	CZ	ARG	A	482	44.146	34.570	24.975	1.00	61.54
ATOM	3781	NH1	ARG	A	482	43.315	33.892	25.763	1.00	57.54
ATOM	3782	NH2	ARG	A	482	44.061	34.429	23.649	1.00	57.68
ATOM	3783	C	ARG	A	482	45.152	38.548	30.949	1.00	45.67
ATOM	3784	O	ARG	A	482	44.113	38.802	31.537	1.00	45.14
ATOM	3785	N	GLU	A	483	46.266	38.212	31.587	1.00	47.81
ATOM	3786	CA	GLU	A	483	46.302	38.113	33.046	1.00	49.80
ATOM	3787	CB	GLU	A	483	47.553	37.348	33.475	1.00	54.17
ATOM	3788	CG	GLU	A	483	47.409	35.855	33.366	1.00	68.42
ATOM	3789	CD	GLU	A	483	46.639	35.276	34.538	1.00	73.82
ATOM	3790	OE1	GLU	A	483	46.280	34.079	34.479	1.00	77.54
ATOM	3791	OE2	GLU	A	483	46.403	36.023	35.518	1.00	76.57
ATOM	3792	C	GLU	A	483	46.249	39.430	33.832	1.00	46.79
ATOM	3793	O	GLU	A	483	45.429	39.598	34.732	1.00	46.86
ATOM	3794	N	ILE	A	484	47.131	40.358	33.492	1.00	46.07
ATOM	3795	CA	ILE	A	484	47.229	41.634	34.203	1.00	44.32
ATOM	3796	CB	ILE	A	484	48.663	42.206	34.073	1.00	45.35
ATOM	3797	CG2	ILE	A	484	48.795	43.470	34.899	1.00	45.15
ATOM	3798	CG1	ILE	A	484	49.680	41.144	34.518	1.00	49.05
ATOM	3799	CD1	ILE	A	484	51.149	41.457	34.192	1.00	46.75
ATOM	3800	C	ILE	A	484	46.249	42.719	33.777	1.00	42.43
ATOM	3801	O	ILE	A	484	45.641	43.381	34.616	1.00	40.91
ATOM	3802	N	VAL	A	485	46.086	42.883	32.470	1.00	43.50
ATOM	3803	CA	VAL	A	485	45.224	43.929	31.935	1.00	41.60
ATOM	3804	CB	VAL	A	485	45.855	44.487	30.637	1.00	41.27

169/396

Figure 2A-69

ATOM	3805	CG1	VAL	A	485	45.172	45.807	30.202	1.00	39.15
ATOM	3806	CG2	VAL	A	485	47.341	44.682	30.865	1.00	38.11
ATOM	3807	C	VAL	A	485	43.804	43.469	31.660	1.00	41.40
ATOM	3808	O	VAL	A	485	42.876	44.270	31.658	1.00	39.92
ATOM	3809	N	GLY	A	486	43.644	42.169	31.432	1.00	44.10
ATOM	3810	CA	GLY	A	486	42.332	41.626	31.136	1.00	40.99
ATOM	3811	C	GLY	A	486	41.929	42.048	29.735	1.00	42.03
ATOM	3812	O	GLY	A	486	40.795	42.468	29.500	1.00	45.45
ATOM	3813	N	VAL	A	487	42.870	41.943	28.806	1.00	40.92
ATOM	3814	CA	VAL	A	487	42.653	42.327	27.414	1.00	41.92
ATOM	3815	CB	VAL	A	487	43.411	43.654	27.088	1.00	43.87
ATOM	3816	CG1	VAL	A	487	43.403	43.938	25.587	1.00	44.94
ATOM	3817	CG2	VAL	A	487	42.750	44.815	27.830	1.00	42.93
ATOM	3818	C	VAL	A	487	43.206	41.199	26.568	1.00	42.82
ATOM	3819	O	VAL	A	487	44.273	40.664	26.891	1.00	44.28
ATOM	3820	N	VAL	A	488	42.480	40.825	25.511	1.00	41.30
ATOM	3821	CA	VAL	A	488	42.896	39.744	24.619	1.00	40.38
ATOM	3822	CB	VAL	A	488	41.902	38.540	24.602	1.00	44.30
ATOM	3823	CG1	VAL	A	488	42.301	37.512	25.613	1.00	49.37
ATOM	3824	CG2	VAL	A	488	40.494	39.020	24.817	1.00	38.39
ATOM	3825	C	VAL	A	488	43.022	40.150	23.163	1.00	42.64
ATOM	3826	O	VAL	A	488	42.169	40.864	22.623	1.00	40.94
ATOM	3827	N	GLU	A	489	44.063	39.630	22.524	1.00	41.61
ATOM	3828	CA	GLU	A	489	44.319	39.905	21.130	1.00	44.48
ATOM	3829	CB	GLU	A	489	45.667	39.313	20.726	1.00	43.24
ATOM	3830	CG	GLU	A	489	45.707	37.792	20.630	1.00	48.79
ATOM	3831	CD	GLU	A	489	45.768	37.084	21.978	1.00	54.53
ATOM	3832	OE1	GLU	A	489	46.012	35.862	21.975	1.00	57.18
ATOM	3833	OE2	GLU	A	489	45.571	37.726	23.035	1.00	56.21
ATOM	3834	C	GLU	A	489	43.187	39.283	20.298	1.00	47.85
ATOM	3835	O	GLU	A	489	42.749	38.172	20.578	1.00	48.35
ATOM	3836	N	PRO	A	490	42.697	40.007	19.276	1.00	48.14
ATOM	3837	CD	PRO	A	490	43.095	41.402	19.016	1.00	49.82
ATOM	3838	CA	PRO	A	490	41.615	39.596	18.370	1.00	48.40
ATOM	3839	CB	PRO	A	490	41.306	40.870	17.577	1.00	50.13
ATOM	3840	CG	PRO	A	490	41.825	41.986	18.456	1.00	53.03
ATOM	3841	C	PRO	A	490	42.039	38.474	17.443	1.00	47.92
ATOM	3842	O	PRO	A	490	41.232	37.633	17.062	1.00	46.79
ATOM	3843	N	VAL	A	491	43.317	38.497	17.084	1.00	49.03
ATOM	3844	CA	VAL	A	491	43.942	37.529	16.196	1.00	48.63
ATOM	3845	CB	VAL	A	491	44.463	38.217	14.933	1.00	49.67
ATOM	3846	CG1	VAL	A	491	45.026	37.192	13.992	1.00	56.76
ATOM	3847	CG2	VAL	A	491	43.352	39.013	14.270	1.00	53.61
ATOM	3848	C	VAL	A	491	45.150	36.945	16.907	1.00	49.07
ATOM	3849	O	VAL	A	491	45.799	37.632	17.687	1.00	49.02
ATOM	3850	N	PRO	A	492	45.472	35.670	16.656	1.00	48.92
ATOM	3851	CD	PRO	A	492	44.716	34.579	16.018	1.00	46.62
ATOM	3852	CA	PRO	A	492	46.648	35.159	17.359	1.00	48.61
ATOM	3853	CB	PRO	A	492	46.476	33.640	17.263	1.00	48.22
ATOM	3854	CG	PRO	A	492	45.720	33.467	15.983	1.00	48.23
ATOM	3855	C	PRO	A	492	47.910	35.682	16.676	1.00	48.49
ATOM	3856	O	PRO	A	492	47.950	35.814	15.456	1.00	48.27
ATOM	3857	N	HIS	A	493	48.930	35.990	17.471	1.00	48.64
ATOM	3858	CA	HIS	A	493	50.185	36.521	16.952	1.00	50.06
ATOM	3859	CB	HIS	A	493	50.420	37.932	17.502	1.00	48.93
ATOM	3860	CG	HIS	A	493	49.526	38.971	16.906	1.00	51.27

170/396

Figure 2A-70

ATOM	3861	CD2	HIS	A	493	49.449	40.307	17.111	1.00	49.23
ATOM	3862	ND1	HIS	A	493	48.569	38.675	15.960	1.00	51.66
ATOM	3863	CE1	HIS	A	493	47.942	39.781	15.609	1.00	45.34
ATOM	3864	NE2	HIS	A	493	48.457	40.787	16.294	1.00	51.79
ATOM	3865	C	HIS	A	493	51.402	35.662	17.296	1.00	50.51
ATOM	3866	O	HIS	A	493	51.691	35.436	18.463	1.00	49.54
ATOM	3867	N	ASP	A	494	52.133	35.218	16.279	1.00	51.92
ATOM	3868	CA	ASP	A	494	53.321	34.409	16.519	1.00	54.02
ATOM	3869	CB	ASP	A	494	53.549	33.427	15.357	1.00	52.42
ATOM	3870	CG	ASP	A	494	53.831	34.121	14.045	1.00	55.77
ATOM	3871	OD1	ASP	A	494	53.980	33.418	13.029	1.00	59.87
ATOM	3872	OD2	ASP	A	494	53.915	35.365	14.019	1.00	60.80
ATOM	3873	C	ASP	A	494	54.535	35.326	16.732	1.00	54.72
ATOM	3874	O	ASP	A	494	54.380	36.547	16.819	1.00	53.54
ATOM	3875	N	GLU	A	495	55.734	34.748	16.809	1.00	54.30
ATOM	3876	CA	GLU	A	495	56.942	35.533	17.064	1.00	54.59
ATOM	3877	CB	GLU	A	495	58.067	34.616	17.534	1.00	53.46
ATOM	3878	CG	GLU	A	495	57.680	33.842	18.790	1.00	55.11
ATOM	3879	CD	GLU	A	495	57.229	34.747	19.915	1.00	56.99
ATOM	3880	OE1	GLU	A	495	56.392	34.318	20.742	1.00	57.63
ATOM	3881	OE2	GLU	A	495	57.725	35.889	19.981	1.00	58.65
ATOM	3882	C	GLU	A	495	57.402	36.386	15.893	1.00	53.54
ATOM	3883	O	GLU	A	495	58.441	37.045	15.943	1.00	53.49
ATOM	3884	N	THR	A	496	56.598	36.381	14.845	1.00	52.16
ATOM	3885	CA	THR	A	496	56.873	37.161	13.661	1.00	50.18
ATOM	3886	CB	THR	A	496	56.105	36.532	12.495	1.00	51.62
ATOM	3887	OG1	THR	A	496	57.015	35.720	11.729	1.00	51.72
ATOM	3888	CG2	THR	A	496	55.460	37.569	11.642	1.00	49.76
ATOM	3889	C	THR	A	496	56.478	38.631	13.923	1.00	48.08
ATOM	3890	O	THR	A	496	57.018	39.561	13.322	1.00	48.74
ATOM	3891	N	TYR	A	497	55.556	38.815	14.858	1.00	45.79
ATOM	3892	CA	TYR	A	497	55.064	40.125	15.259	1.00	45.41
ATOM	3893	CB	TYR	A	497	53.648	40.005	15.812	1.00	40.90
ATOM	3894	CG	TYR	A	497	52.571	39.690	14.814	1.00	43.52
ATOM	3895	CD1	TYR	A	497	51.709	40.683	14.357	1.00	40.95
ATOM	3896	CE1	TYR	A	497	50.657	40.383	13.511	1.00	43.27
ATOM	3897	CD2	TYR	A	497	52.357	38.382	14.384	1.00	45.30
ATOM	3898	CE2	TYR	A	497	51.311	38.070	13.541	1.00	42.64
ATOM	3899	CZ	TYR	A	497	50.459	39.071	13.113	1.00	47.05
ATOM	3900	OH	TYR	A	497	49.369	38.737	12.349	1.00	49.11
ATOM	3901	C	TYR	A	497	55.917	40.728	16.368	1.00	45.99
ATOM	3902	O	TYR	A	497	56.750	40.053	16.967	1.00	47.34
ATOM	3903	N	CYS	A	498	55.682	42.004	16.641	1.00	45.70
ATOM	3904	CA	CYS	A	498	56.359	42.710	17.718	1.00	47.45
ATOM	3905	CB	CYS	A	498	57.641	43.392	17.267	1.00	45.00
ATOM	3906	SG	CYS	A	498	58.620	43.866	18.724	1.00	55.28
ATOM	3907	C	CYS	A	498	55.372	43.762	18.155	1.00	47.37
ATOM	3908	O	CYS	A	498	55.583	44.960	17.962	1.00	49.07
ATOM	3909	N	ASP	A	499	54.281	43.297	18.744	1.00	45.67
ATOM	3910	CA	ASP	A	499	53.213	44.178	19.176	1.00	44.56
ATOM	3911	CB	ASP	A	499	52.073	43.325	19.695	1.00	45.58
ATOM	3912	CG	ASP	A	499	51.460	42.482	18.590	1.00	46.64
ATOM	3913	OD1	ASP	A	499	50.766	41.497	18.900	1.00	45.92
ATOM	3914	OD2	ASP	A	499	51.684	42.821	17.404	1.00	46.25
ATOM	3915	C	ASP	A	499	53.586	45.285	20.149	1.00	44.34
ATOM	3916	O	ASP	A	499	53.026	46.359	20.091	1.00	45.57

171/396

Figure 2A-71

ATOM	3917	N	PRO	A	500	54.530	45.043	21.064	1.00	46.31
ATOM	3918	CD	PRO	A	500	55.153	43.794	21.534	1.00	43.79
ATOM	3919	CA	PRO	A	500	54.844	46.167	21.957	1.00	44.28
ATOM	3920	CB	PRO	A	500	55.752	45.533	23.023	1.00	44.46
ATOM	3921	CG	PRO	A	500	56.315	44.321	22.344	1.00	48.32
ATOM	3922	C	PRO	A	500	55.517	47.319	21.206	1.00	42.60
ATOM	3923	O	PRO	A	500	55.285	48.493	21.508	1.00	41.01
ATOM	3924	N	ALA	A	501	56.323	46.978	20.207	1.00	42.68
ATOM	3925	CA	ALA	A	501	57.037	47.977	19.413	1.00	42.27
ATOM	3926	CB	ALA	A	501	58.091	47.297	18.559	1.00	42.68
ATOM	3927	C	ALA	A	501	56.123	48.835	18.531	1.00	42.39
ATOM	3928	O	ALA	A	501	56.558	49.851	17.975	1.00	42.53
ATOM	3929	N	SER	A	502	54.862	48.441	18.402	1.00	42.19
ATOM	3930	CA	SER	A	502	53.937	49.210	17.579	1.00	44.34
ATOM	3931	CB	SER	A	502	52.769	48.344	17.122	1.00	42.47
ATOM	3932	OG	SER	A	502	51.765	48.322	18.119	1.00	44.34
ATOM	3933	C	SER	A	502	53.405	50.386	18.395	1.00	43.47
ATOM	3934	O	SER	A	502	52.462	51.065	17.999	1.00	40.87
ATOM	3935	N	LEU	A	503	54.006	50.595	19.558	1.00	44.78
ATOM	3936	CA	LEU	A	503	53.637	51.694	20.439	1.00	42.25
ATOM	3937	CB	LEU	A	503	53.484	51.196	21.883	1.00	44.72
ATOM	3938	CG	LEU	A	503	52.682	51.995	22.917	1.00	46.69
ATOM	3939	CD1	LEU	A	503	53.507	52.133	24.176	1.00	47.05
ATOM	3940	CD2	LEU	A	503	52.288	53.361	22.389	1.00	45.50
ATOM	3941	C	LEU	A	503	54.810	52.661	20.365	1.00	39.10
ATOM	3942	O	LEU	A	503	55.963	52.236	20.466	1.00	38.56
ATOM	3943	N	PHE	A	504	54.512	53.946	20.200	1.00	35.85
ATOM	3944	CA	PHE	A	504	55.533	54.987	20.120	1.00	38.30
ATOM	3945	CB	PHE	A	504	54.877	56.366	20.292	1.00	35.28
ATOM	3946	CG	PHE	A	504	55.867	57.509	20.343	1.00	36.50
ATOM	3947	CD1	PHE	A	504	56.427	58.013	19.181	1.00	36.05
ATOM	3948	CD2	PHE	A	504	56.258	58.052	21.559	1.00	35.02
ATOM	3949	CE1	PHE	A	504	57.363	59.042	19.219	1.00	37.56
ATOM	3950	CE2	PHE	A	504	57.190	59.076	21.617	1.00	36.75
ATOM	3951	CZ	PHE	A	504	57.750	59.578	20.445	1.00	38.63
ATOM	3952	C	PHE	A	504	56.714	54.865	21.113	1.00	37.03
ATOM	3953	O	PHE	A	504	57.875	54.787	20.709	1.00	39.31
ATOM	3954	N	HIS	A	505	56.422	54.833	22.403	1.00	38.76
ATOM	3955	CA	HIS	A	505	57.492	54.781	23.400	1.00	41.61
ATOM	3956	CB	HIS	A	505	56.886	54.876	24.791	1.00	39.74
ATOM	3957	CG	HIS	A	505	55.874	55.965	24.919	1.00	42.45
ATOM	3958	CD2	HIS	A	505	54.651	56.112	24.355	1.00	42.32
ATOM	3959	ND1	HIS	A	505	56.070	57.078	25.710	1.00	44.33
ATOM	3960	CE1	HIS	A	505	55.009	57.863	25.629	1.00	43.14
ATOM	3961	NE2	HIS	A	505	54.134	57.299	24.814	1.00	40.08
ATOM	3962	C	HIS	A	505	58.400	53.564	23.306	1.00	41.93
ATOM	3963	O	HIS	A	505	59.583	53.637	23.667	1.00	40.05
ATOM	3964	N	VAL	A	506	57.865	52.449	22.808	1.00	39.41
ATOM	3965	CA	VAL	A	506	58.689	51.257	22.689	1.00	38.72
ATOM	3966	CB	VAL	A	506	57.817	49.977	22.533	1.00	40.10
ATOM	3967	CG1	VAL	A	506	58.682	48.783	22.215	1.00	38.77
ATOM	3968	CG2	VAL	A	506	57.040	49.709	23.824	1.00	37.88
ATOM	3969	C	VAL	A	506	59.649	51.387	21.515	1.00	40.00
ATOM	3970	O	VAL	A	506	60.857	51.285	21.689	1.00	39.53
ATOM	3971	N	SER	A	507	59.128	51.617	20.311	1.00	40.83
ATOM	3972	CA	SER	A	507	60.014	51.746	19.162	1.00	40.63

172/396

Figure 2A-72

ATOM	3973	CB	SER	A	507	59.217	51.654	17.852	1.00	41.52
ATOM	3974	OG	SER	A	507	58.135	52.555	17.878	1.00	48.67
ATOM	3975	C	SER	A	507	60.823	53.042	19.182	1.00	39.78
ATOM	3976	O	SER	A	507	61.775	53.179	18.420	1.00	41.92
ATOM	3977	N	ASN	A	508	60.454	53.995	20.036	1.00	40.20
ATOM	3978	CA	ASN	A	508	61.212	55.248	20.110	1.00	42.40
ATOM	3979	CB	ASN	A	508	60.265	56.453	19.982	1.00	41.95
ATOM	3980	CG	ASN	A	508	59.836	56.678	18.523	1.00	46.71
ATOM	3981	OD1	ASN	A	508	60.527	57.355	17.762	1.00	46.90
ATOM	3982	ND2	ASN	A	508	58.724	56.059	18.120	1.00	45.34
ATOM	3983	C	ASN	A	508	62.116	55.336	21.336	1.00	43.34
ATOM	3984	O	ASN	A	508	62.608	56.403	21.710	1.00	41.04
ATOM	3985	N	ASP	A	509	62.318	54.187	21.971	1.00	45.00
ATOM	3986	CA	ASP	A	509	63.249	54.074	23.083	1.00	42.33
ATOM	3987	CB	ASP	A	509	64.654	54.215	22.477	1.00	41.53
ATOM	3988	CG	ASP	A	509	65.764	54.010	23.489	1.00	46.22
ATOM	3989	OD1	ASP	A	509	65.685	53.039	24.269	1.00	42.55
ATOM	3990	OD2	ASP	A	509	66.725	54.815	23.486	1.00	46.13
ATOM	3991	C	ASP	A	509	63.077	55.001	24.301	1.00	43.81
ATOM	3992	O	ASP	A	509	64.058	55.588	24.781	1.00	45.29
ATOM	3993	N	TYR	A	510	61.848	55.122	24.808	1.00	41.95
ATOM	3994	CA	TYR	A	510	61.560	55.940	26.000	1.00	40.08
ATOM	3995	CB	TYR	A	510	60.464	56.980	25.724	1.00	40.11
ATOM	3996	CG	TYR	A	510	60.919	58.157	24.887	1.00	48.70
ATOM	3997	CD1	TYR	A	510	61.730	59.156	25.433	1.00	51.95
ATOM	3998	CE1	TYR	A	510	62.191	60.226	24.645	1.00	55.29
ATOM	3999	CD2	TYR	A	510	60.575	58.254	23.537	1.00	48.78
ATOM	4000	CE2	TYR	A	510	61.026	59.311	22.746	1.00	50.58
ATOM	4001	CZ	TYR	A	510	61.835	60.293	23.306	1.00	54.68
ATOM	4002	OH	TYR	A	510	62.283	61.338	22.527	1.00	54.66
ATOM	4003	C	TYR	A	510	61.052	55.021	27.101	1.00	42.21
ATOM	4004	O	TYR	A	510	60.280	54.090	26.834	1.00	40.78
ATOM	4005	N	SER	A	511	61.471	55.269	28.338	1.00	40.44
ATOM	4006	CA	SER	A	511	61.007	54.445	29.432	1.00	40.80
ATOM	4007	CB	SER	A	511	61.839	54.690	30.704	1.00	44.14
ATOM	4008	OG	SER	A	511	61.731	56.029	31.132	1.00	46.61
ATOM	4009	C	SER	A	511	59.546	54.801	29.650	1.00	40.20
ATOM	4010	O	SER	A	511	59.130	55.928	29.390	1.00	39.15
ATOM	4011	N	PHE	A	512	58.784	53.844	30.177	1.00	39.73
ATOM	4012	CA	PHE	A	512	57.357	54.000	30.370	1.00	37.19
ATOM	4013	CB	PHE	A	512	56.669	52.859	29.605	1.00	41.14
ATOM	4014	CG	PHE	A	512	55.326	53.218	29.012	1.00	41.40
ATOM	4015	CD1	PHE	A	512	54.153	52.628	29.494	1.00	39.71
ATOM	4016	CD2	PHE	A	512	55.238	54.106	27.945	1.00	38.91
ATOM	4017	CE1	PHE	A	512	52.896	52.916	28.913	1.00	40.42
ATOM	4018	CE2	PHE	A	512	53.997	54.404	27.354	1.00	40.81
ATOM	4019	CZ	PHE	A	512	52.819	53.804	27.842	1.00	41.09
ATOM	4020	C	PHE	A	512	56.841	54.037	31.808	1.00	40.06
ATOM	4021	O	PHE	A	512	55.772	54.591	32.052	1.00	38.81
ATOM	4022	N	ILE	A	513	57.585	53.487	32.772	1.00	39.93
ATOM	4023	CA	ILE	A	513	57.093	53.449	34.160	1.00	37.50
ATOM	4024	CB	ILE	A	513	58.097	52.691	35.090	1.00	39.26
ATOM	4025	CG2	ILE	A	513	59.253	53.605	35.488	1.00	34.72
ATOM	4026	CG1	ILE	A	513	57.379	52.217	36.357	1.00	40.27
ATOM	4027	CD1	ILE	A	513	56.249	51.213	36.113	1.00	42.83
ATOM	4028	C	ILE	A	513	56.751	54.810	34.780	1.00	35.68

173/396

Figure 2A-73

ATOM	4029	O	ILE	A	513	55.939	54.896	35.695	1.00	38.62
ATOM	4030	N	ARG	A	514	57.349	55.875	34.265	1.00	38.42
ATOM	4031	CA	ARG	A	514	57.101	57.239	34.764	1.00	40.36
ATOM	4032	CB	ARG	A	514	57.894	58.249	33.917	1.00	44.12
ATOM	4033	CG	ARG	A	514	57.480	58.251	32.439	1.00	49.25
ATOM	4034	CD	ARG	A	514	58.521	58.931	31.580	1.00	52.45
ATOM	4035	NE	ARG	A	514	58.786	60.266	32.076	1.00	60.64
ATOM	4036	CZ	ARG	A	514	59.832	61.001	31.723	1.00	63.17
ATOM	4037	NH1	ARG	A	514	60.720	60.518	30.861	1.00	58.03
ATOM	4038	NH2	ARG	A	514	59.991	62.216	32.247	1.00	62.43
ATOM	4039	C	ARG	A	514	55.628	57.622	34.747	1.00	39.98
ATOM	4040	O	ARG	A	514	55.179	58.426	35.562	1.00	41.11
ATOM	4041	N	TYR	A	515	54.860	57.058	33.818	1.00	41.34
ATOM	4042	CA	TYR	A	515	53.432	57.388	33.763	1.00	39.91
ATOM	4043	CB	TYR	A	515	52.843	56.964	32.398	1.00	40.49
ATOM	4044	CG	TYR	A	515	53.501	57.694	31.225	1.00	36.15
ATOM	4045	CD1	TYR	A	515	53.274	59.045	31.006	1.00	36.85
ATOM	4046	CE1	TYR	A	515	53.938	59.735	29.986	1.00	35.57
ATOM	4047	CD2	TYR	A	515	54.406	57.046	30.394	1.00	37.78
ATOM	4048	CE2	TYR	A	515	55.074	57.721	29.395	1.00	35.94
ATOM	4049	CZ	TYR	A	515	54.831	59.067	29.193	1.00	37.80
ATOM	4050	OH	TYR	A	515	55.475	59.722	28.173	1.00	39.95
ATOM	4051	C	TYR	A	515	52.721	56.710	34.927	1.00	38.20
ATOM	4052	O	TYR	A	515	51.674	57.163	35.392	1.00	40.17
ATOM	4053	N	TYR	A	516	53.296	55.612	35.405	1.00	39.06
ATOM	4054	CA	TYR	A	516	52.728	54.912	36.555	1.00	39.00
ATOM	4055	CB	TYR	A	516	53.332	53.506	36.701	1.00	39.39
ATOM	4056	CG	TYR	A	516	52.699	52.700	37.813	1.00	37.55
ATOM	4057	CD1	TYR	A	516	51.551	51.940	37.585	1.00	36.91
ATOM	4058	CE1	TYR	A	516	50.909	51.267	38.630	1.00	39.92
ATOM	4059	CD2	TYR	A	516	53.208	52.763	39.118	1.00	39.51
ATOM	4060	CE2	TYR	A	516	52.585	52.093	40.170	1.00	38.71
ATOM	4061	CZ	TYR	A	516	51.435	51.351	39.924	1.00	42.83
ATOM	4062	OH	TYR	A	516	50.804	50.714	40.972	1.00	45.08
ATOM	4063	C	TYR	A	516	53.046	55.730	37.810	1.00	37.90
ATOM	4064	O	TYR	A	516	52.141	56.117	38.539	1.00	41.39
ATOM	4065	N	THR	A	517	54.322	56.037	38.039	1.00	37.66
ATOM	4066	CA	THR	A	517	54.689	56.790	39.243	1.00	40.70
ATOM	4067	CB	THR	A	517	56.215	56.869	39.420	1.00	38.04
ATOM	4068	OG1	THR	A	517	56.803	57.492	38.272	1.00	39.55
ATOM	4069	CG2	THR	A	517	56.800	55.457	39.607	1.00	38.31
ATOM	4070	C	THR	A	517	54.116	58.204	39.328	1.00	40.88
ATOM	4071	O	THR	A	517	53.673	58.645	40.392	1.00	39.53
ATOM	4072	N	ARG	A	518	54.112	58.914	38.206	1.00	44.33
ATOM	4073	CA	ARG	A	518	53.584	60.278	38.171	1.00	41.60
ATOM	4074	CB	ARG	A	518	53.741	60.823	36.757	1.00	47.03
ATOM	4075	CG	ARG	A	518	53.145	62.194	36.509	1.00	49.97
ATOM	4076	CD	ARG	A	518	52.394	62.158	35.192	1.00	59.51
ATOM	4077	NE	ARG	A	518	50.971	61.934	35.398	1.00	61.52
ATOM	4078	CZ	ARG	A	518	50.119	61.586	34.439	1.00	64.28
ATOM	4079	NH1	ARG	A	518	48.830	61.414	34.733	1.00	62.51
ATOM	4080	NH2	ARG	A	518	50.559	61.386	33.199	1.00	58.75
ATOM	4081	C	ARG	A	518	52.120	60.296	38.618	1.00	40.37
ATOM	4082	O	ARG	A	518	51.697	61.166	39.393	1.00	37.89
ATOM	4083	N	THR	A	519	51.353	59.309	38.152	1.00	39.75
ATOM	4084	CA	THR	A	519	49.944	59.187	38.513	1.00	40.37

174/396

Figure 2A-74

ATOM	4085	CB	THR	A	519	49.260	57.972	37.833	1.00	42.05
ATOM	4086	OG1	THR	A	519	49.415	58.050	36.410	1.00	39.88
ATOM	4087	CG2	THR	A	519	47.788	57.941	38.204	1.00	38.20
ATOM	4088	C	THR	A	519	49.792	59.000	40.020	1.00	42.04
ATOM	4089	O	THR	A	519	48.957	59.643	40.654	1.00	41.80
ATOM	4090	N	LEU	A	520	50.567	58.097	40.605	1.00	42.75
ATOM	4091	CA	LEU	A	520	50.448	57.949	42.052	1.00	44.99
ATOM	4092	CB	LEU	A	520	51.203	56.705	42.571	1.00	38.76
ATOM	4093	CG	LEU	A	520	50.431	55.363	42.542	1.00	45.27
ATOM	4094	CD1	LEU	A	520	50.108	54.966	41.068	1.00	42.43
ATOM	4095	CD2	LEU	A	520	51.268	54.230	43.215	1.00	36.72
ATOM	4096	C	LEU	A	520	50.948	59.229	42.738	1.00	43.27
ATOM	4097	O	LEU	A	520	50.363	59.654	43.727	1.00	46.87
ATOM	4098	N	TYR	A	521	51.995	59.871	42.221	1.00	42.07
ATOM	4099	CA	TYR	A	521	52.459	61.099	42.888	1.00	41.54
ATOM	4100	CB	TYR	A	521	53.735	61.674	42.273	1.00	37.83
ATOM	4101	CG	TYR	A	521	54.931	60.790	42.296	1.00	39.57
ATOM	4102	CD1	TYR	A	521	55.107	59.828	43.297	1.00	39.02
ATOM	4103	CE1	TYR	A	521	56.241	59.032	43.318	1.00	38.52
ATOM	4104	CD2	TYR	A	521	55.918	60.924	41.324	1.00	36.73
ATOM	4105	CE2	TYR	A	521	57.040	60.138	41.343	1.00	37.74
ATOM	4106	CZ	TYR	A	521	57.201	59.196	42.338	1.00	38.68
ATOM	4107	OH	TYR	A	521	58.347	58.437	42.340	1.00	43.27
ATOM	4108	C	TYR	A	521	51.429	62.208	42.848	1.00	41.11
ATOM	4109	O	TYR	A	521	51.169	62.860	43.867	1.00	42.38
ATOM	4110	N	GLN	A	522	50.825	62.428	41.680	1.00	41.47
ATOM	4111	CA	GLN	A	522	49.855	63.509	41.588	1.00	40.68
ATOM	4112	CB	GLN	A	522	49.251	63.605	40.173	1.00	40.63
ATOM	4113	CG	GLN	A	522	48.088	62.702	39.840	1.00	44.10
ATOM	4114	CD	GLN	A	522	47.673	62.861	38.378	1.00	46.60
ATOM	4115	OE1	GLN	A	522	48.418	62.501	37.478	1.00	46.40
ATOM	4116	NE2	GLN	A	522	46.490	63.432	38.144	1.00	47.31
ATOM	4117	C	GLN	A	522	48.762	63.438	42.633	1.00	40.69
ATOM	4118	O	GLN	A	522	48.330	64.468	43.157	1.00	42.82
ATOM	4119	N	PHE	A	523	48.296	62.243	42.967	1.00	40.34
ATOM	4120	CA	PHE	A	523	47.237	62.208	43.962	1.00	42.14
ATOM	4121	CB	PHE	A	523	46.353	60.964	43.755	1.00	43.96
ATOM	4122	CG	PHE	A	523	45.489	61.055	42.513	1.00	42.91
ATOM	4123	CD1	PHE	A	523	44.490	62.019	42.423	1.00	40.63
ATOM	4124	CD2	PHE	A	523	45.720	60.226	41.414	1.00	45.42
ATOM	4125	CE1	PHE	A	523	43.725	62.169	41.255	1.00	43.02
ATOM	4126	CE2	PHE	A	523	44.960	60.365	40.235	1.00	47.65
ATOM	4127	CZ	PHE	A	523	43.958	61.347	40.163	1.00	43.01
ATOM	4128	C	PHE	A	523	47.767	62.355	45.389	1.00	39.37
ATOM	4129	O	PHE	A	523	47.063	62.846	46.263	1.00	38.85
ATOM	4130	N	GLN	A	524	49.017	61.966	45.611	1.00	41.23
ATOM	4131	CA	GLN	A	524	49.629	62.130	46.935	1.00	43.15
ATOM	4132	CB	GLN	A	524	50.993	61.423	46.999	1.00	41.93
ATOM	4133	CG	GLN	A	524	50.889	59.898	46.972	1.00	43.92
ATOM	4134	CD	GLN	A	524	52.245	59.213	47.045	1.00	47.95
ATOM	4135	OE1	GLN	A	524	52.972	59.354	48.033	1.00	52.23
ATOM	4136	NE2	GLN	A	524	52.594	58.475	46.003	1.00	41.17
ATOM	4137	C	GLN	A	524	49.798	63.638	47.153	1.00	42.66
ATOM	4138	O	GLN	A	524	49.434	64.161	48.200	1.00	43.56
ATOM	4139	N	PHE	A	525	50.327	64.333	46.145	1.00	43.40
ATOM	4140	CA	PHE	A	525	50.499	65.773	46.224	1.00	39.85

175/396

Figure 2A-75

ATOM	4141	CB	PHE	A	525	51.049	66.376	44.923	1.00	39.52
ATOM	4142	CG	PHE	A	525	52.425	65.942	44.575	1.00	40.24
ATOM	4143	CD1	PHE	A	525	53.219	65.262	45.494	1.00	40.18
ATOM	4144	CD2	PHE	A	525	52.933	66.195	43.305	1.00	40.63
ATOM	4145	CE1	PHE	A	525	54.504	64.830	45.150	1.00	39.70
ATOM	4146	CE2	PHE	A	525	54.211	65.771	42.952	1.00	42.85
ATOM	4147	CZ	PHE	A	525	55.002	65.079	43.885	1.00	41.79
ATOM	4148	C	PHE	A	525	49.153	66.412	46.456	1.00	44.45
ATOM	4149	O	PHE	A	525	49.006	67.255	47.356	1.00	47.58
ATOM	4150	N	GLN	A	526	48.164	66.031	45.642	1.00	44.63
ATOM	4151	CA	GLN	A	526	46.833	66.631	45.760	1.00	42.75
ATOM	4152	CB	GLN	A	526	45.904	66.167	44.623	1.00	45.63
ATOM	4153	CG	GLN	A	526	44.551	66.913	44.554	1.00	42.95
ATOM	4154	CD	GLN	A	526	44.708	68.395	44.180	1.00	46.60
ATOM	4155	OE1	GLN	A	526	43.727	69.101	43.919	1.00	49.87
ATOM	4156	NE2	GLN	A	526	45.944	68.863	44.153	1.00	46.62
ATOM	4157	C	GLN	A	526	46.163	66.375	47.098	1.00	40.47
ATOM	4158	O	GLN	A	526	45.517	67.273	47.645	1.00	41.53
ATOM	4159	N	GLU	A	527	46.275	65.162	47.627	1.00	40.32
ATOM	4160	CA	GLU	A	527	45.655	64.897	48.927	1.00	42.97
ATOM	4161	CB	GLU	A	527	45.778	63.419	49.320	1.00	44.07
ATOM	4162	CG	GLU	A	527	44.906	63.048	50.520	1.00	49.35
ATOM	4163	CD	GLU	A	527	44.837	61.544	50.768	1.00	57.01
ATOM	4164	OE1	GLU	A	527	45.824	60.974	51.289	1.00	60.89
ATOM	4165	OE2	GLU	A	527	43.794	60.930	50.432	1.00	58.90
ATOM	4166	C	GLU	A	527	46.364	65.779	49.960	1.00	44.14
ATOM	4167	O	GLU	A	527	45.718	66.430	50.783	1.00	46.34
ATOM	4168	N	ALA	A	528	47.690	65.839	49.868	1.00	43.48
ATOM	4169	CA	ALA	A	528	48.483	66.645	50.788	1.00	46.38
ATOM	4170	CB	ALA	A	528	49.964	66.441	50.510	1.00	46.10
ATOM	4171	C	ALA	A	528	48.139	68.131	50.734	1.00	47.76
ATOM	4172	O	ALA	A	528	47.872	68.749	51.767	1.00	49.43
ATOM	4173	N	LEU	A	529	48.144	68.721	49.542	1.00	50.02
ATOM	4174	CA	LEU	A	529	47.825	70.139	49.440	1.00	48.74
ATOM	4175	CB	LEU	A	529	48.039	70.661	48.013	1.00	49.61
ATOM	4176	CG	LEU	A	529	49.471	70.939	47.525	1.00	49.91
ATOM	4177	CD1	LEU	A	529	50.449	71.015	48.699	1.00	49.08
ATOM	4178	CD2	LEU	A	529	49.896	69.849	46.580	1.00	51.73
ATOM	4179	C	LEU	A	529	46.414	70.441	49.886	1.00	47.73
ATOM	4180	O	LEU	A	529	46.162	71.475	50.480	1.00	50.14
ATOM	4181	N	CYS	A	530	45.484	69.539	49.611	1.00	51.54
ATOM	4182	CA	CYS	A	530	44.099	69.760	50.005	1.00	51.82
ATOM	4183	C	CYS	A	530	43.891	69.643	51.514	1.00	50.77
ATOM	4184	O	CYS	A	530	43.030	70.317	52.083	1.00	48.74
ATOM	4185	CB	CYS	A	530	43.186	68.808	49.229	1.00	55.96
ATOM	4186	SG	CYS	A	530	43.188	69.309	47.479	1.00	65.58
ATOM	4187	N	GLN	A	531	44.653	68.781	52.170	1.00	49.89
ATOM	4188	CA	GLN	A	531	44.526	68.693	53.613	1.00	55.22
ATOM	4189	CB	GLN	A	531	45.292	67.485	54.171	1.00	59.62
ATOM	4190	CG	GLN	A	531	44.586	66.148	53.867	1.00	68.83
ATOM	4191	CD	GLN	A	531	45.120	64.959	54.666	1.00	71.91
ATOM	4192	OE1	GLN	A	531	44.583	63.848	54.576	1.00	69.57
ATOM	4193	NE2	GLN	A	531	46.179	65.188	55.448	1.00	72.85
ATOM	4194	C	GLN	A	531	45.091	70.003	54.160	1.00	57.29
ATOM	4195	O	GLN	A	531	44.555	70.567	55.113	1.00	57.51
ATOM	4196	N	ALA	A	532	46.151	70.502	53.522	1.00	56.65

176/396

Figure 2A-76

ATOM	4197	CA	ALA	A	532	46.780	71.748	53.935	1.00	57.09
ATOM	4198	CB	ALA	A	532	48.126	71.909	53.261	1.00	56.94
ATOM	4199	C	ALA	A	532	45.900	72.930	53.595	1.00	58.31
ATOM	4200	O	ALA	A	532	46.149	74.042	54.055	1.00	61.50
ATOM	4201	N	ALA	A	533	44.874	72.695	52.784	1.00	56.73
ATOM	4202	CA	ALA	A	533	43.963	73.760	52.401	1.00	55.12
ATOM	4203	CB	ALA	A	533	43.681	73.686	50.915	1.00	54.64
ATOM	4204	C	ALA	A	533	42.665	73.654	53.203	1.00	55.56
ATOM	4205	O	ALA	A	533	41.714	74.419	53.001	1.00	53.77
ATOM	4206	N	LYS	A	534	42.634	72.693	54.119	1.00	57.02
ATOM	4207	CA	LYS	A	534	41.467	72.477	54.968	1.00	57.79
ATOM	4208	CB	LYS	A	534	41.176	73.745	55.786	1.00	61.03
ATOM	4209	CG	LYS	A	534	42.416	74.593	56.111	1.00	65.68
ATOM	4210	CD	LYS	A	534	43.166	74.091	57.336	1.00	70.71
ATOM	4211	CE	LYS	A	534	42.507	74.590	58.626	1.00	73.99
ATOM	4212	NZ	LYS	A	534	41.071	74.181	58.760	1.00	76.68
ATOM	4213	C	LYS	A	534	40.228	72.101	54.136	1.00	58.01
ATOM	4214	O	LYS	A	534	39.104	72.482	54.482	1.00	53.80
ATOM	4215	N	HIS	A	535	40.434	71.364	53.039	1.00	56.66
ATOM	4216	CA	HIS	A	535	39.317	70.936	52.194	1.00	55.71
ATOM	4217	CB	HIS	A	535	39.824	70.216	50.945	1.00	54.43
ATOM	4218	CG	HIS	A	535	38.728	69.708	50.064	1.00	50.73
ATOM	4219	CD2	HIS	A	535	38.406	68.452	49.674	1.00	48.93
ATOM	4220	ND1	HIS	A	535	37.788	70.540	49.495	1.00	48.48
ATOM	4221	CE1	HIS	A	535	36.934	69.818	48.792	1.00	49.17
ATOM	4222	NE2	HIS	A	535	37.287	68.548	48.884	1.00	48.79
ATOM	4223	C	HIS	A	535	38.435	69.987	52.997	1.00	56.96
ATOM	4224	O	HIS	A	535	38.945	69.093	53.671	1.00	55.76
ATOM	4225	N	GLU	A	536	37.117	70.157	52.904	1.00	60.03
ATOM	4226	CA	GLU	A	536	36.198	69.330	53.679	1.00	63.33
ATOM	4227	CB	GLU	A	536	35.002	70.172	54.150	1.00	66.23
ATOM	4228	CG	GLU	A	536	35.379	71.434	54.928	1.00	73.51
ATOM	4229	CD	GLU	A	536	35.417	72.679	54.045	1.00	81.21
ATOM	4230	OE1	GLU	A	536	36.117	72.651	53.003	1.00	83.26
ATOM	4231	OE2	GLU	A	536	34.745	73.683	54.393	1.00	82.46
ATOM	4232	C	GLU	A	536	35.668	68.026	53.074	1.00	64.47
ATOM	4233	O	GLU	A	536	35.877	66.943	53.649	1.00	68.21
ATOM	4234	N	GLY	A	537	34.978	68.106	51.940	1.00	59.08
ATOM	4235	CA	GLY	A	537	34.416	66.891	51.367	1.00	57.10
ATOM	4236	C	GLY	A	537	35.317	65.978	50.546	1.00	54.60
ATOM	4237	O	GLY	A	537	36.522	65.897	50.785	1.00	54.54
ATOM	4238	N	PRO	A	538	34.747	65.275	49.555	1.00	51.10
ATOM	4239	CD	PRO	A	538	33.334	65.397	49.157	1.00	52.04
ATOM	4240	CA	PRO	A	538	35.460	64.348	48.664	1.00	49.38
ATOM	4241	CB	PRO	A	538	34.389	63.959	47.637	1.00	50.43
ATOM	4242	CG	PRO	A	538	33.114	64.116	48.386	1.00	52.50
ATOM	4243	C	PRO	A	538	36.675	65.003	47.993	1.00	47.66
ATOM	4244	O	PRO	A	538	36.590	66.120	47.480	1.00	44.58
ATOM	4245	N	LEU	A	539	37.793	64.290	47.981	1.00	43.52
ATOM	4246	CA	LEU	A	539	39.013	64.809	47.393	1.00	44.94
ATOM	4247	CB	LEU	A	539	40.104	63.725	47.417	1.00	41.39
ATOM	4248	CG	LEU	A	539	41.476	64.046	46.848	1.00	43.92
ATOM	4249	CD1	LEU	A	539	42.110	65.203	47.617	1.00	39.43
ATOM	4250	CD2	LEU	A	539	42.359	62.799	46.926	1.00	46.54
ATOM	4251	C	LEU	A	539	38.851	65.364	45.974	1.00	46.49
ATOM	4252	O	LEU	A	539	39.471	66.378	45.647	1.00	43.63

177/396

Figure 2A-77

ATOM	4253	N	HIS	A	540	38.012	64.750	45.134	1.00	46.63
ATOM	4254	CA	HIS	A	540	37.894	65.259	43.759	1.00	48.04
ATOM	4255	CB	HIS	A	540	37.176	64.256	42.835	1.00	46.66
ATOM	4256	CG	HIS	A	540	35.687	64.247	42.965	1.00	46.42
ATOM	4257	CD2	HIS	A	540	34.727	64.818	42.200	1.00	45.95
ATOM	4258	ND1	HIS	A	540	35.026	63.566	43.968	1.00	47.69
ATOM	4259	CE1	HIS	A	540	33.722	63.716	43.811	1.00	47.70
ATOM	4260	NE2	HIS	A	540	33.515	64.471	42.747	1.00	48.43
ATOM	4261	C	HIS	A	540	37.274	66.636	43.587	1.00	47.56
ATOM	4262	O	HIS	A	540	37.359	67.205	42.508	1.00	52.02
ATOM	4263	N	LYS	A	541	36.680	67.190	44.639	1.00	48.99
ATOM	4264	CA	LYS	A	541	36.051	68.510	44.548	1.00	51.25
ATOM	4265	CB	LYS	A	541	34.771	68.545	45.392	1.00	50.92
ATOM	4266	CG	LYS	A	541	33.908	67.301	45.252	1.00	55.12
ATOM	4267	CD	LYS	A	541	32.475	67.639	44.921	1.00	58.74
ATOM	4268	CE	LYS	A	541	31.833	68.463	46.006	1.00	59.61
ATOM	4269	NZ	LYS	A	541	30.392	68.709	45.733	1.00	62.37
ATOM	4270	C	LYS	A	541	36.982	69.612	45.042	1.00	52.92
ATOM	4271	O	LYS	A	541	36.620	70.786	45.054	1.00	52.16
ATOM	4272	N	CYS	A	542	38.187	69.228	45.440	1.00	54.09
ATOM	4273	CA	CYS	A	542	39.133	70.182	45.991	1.00	55.53
ATOM	4274	C	CYS	A	542	39.712	71.228	45.049	1.00	56.59
ATOM	4275	O	CYS	A	542	39.962	70.980	43.867	1.00	55.69
ATOM	4276	CB	CYS	A	542	40.272	69.434	46.686	1.00	56.44
ATOM	4277	SG	CYS	A	542	41.573	70.531	47.331	1.00	60.82
ATOM	4278	N	ASP	A	543	39.922	72.411	45.608	1.00	55.11
ATOM	4279	CA	ASP	A	543	40.503	73.529	44.883	1.00	55.25
ATOM	4280	CB	ASP	A	543	39.408	74.537	44.538	1.00	55.57
ATOM	4281	CG	ASP	A	543	39.911	75.677	43.680	1.00	59.25
ATOM	4282	OD1	ASP	A	543	41.076	75.612	43.215	1.00	59.12
ATOM	4283	OD2	ASP	A	543	39.132	76.634	43.466	1.00	59.02
ATOM	4284	C	ASP	A	543	41.522	74.131	45.854	1.00	53.44
ATOM	4285	O	ASP	A	543	41.167	74.509	46.968	1.00	55.06
ATOM	4286	N	ILE	A	544	42.785	74.211	45.459	1.00	52.90
ATOM	4287	CA	ILE	A	544	43.782	74.748	46.377	1.00	54.53
ATOM	4288	CB	ILE	A	544	45.162	74.127	46.131	1.00	52.70
ATOM	4289	CG2	ILE	A	544	45.053	72.628	46.200	1.00	54.41
ATOM	4290	CG1	ILE	A	544	45.709	74.562	44.773	1.00	51.08
ATOM	4291	CD1	ILE	A	544	47.164	74.173	44.557	1.00	50.53
ATOM	4292	C	ILE	A	544	43.950	76.266	46.392	1.00	56.56
ATOM	4293	O	ILE	A	544	44.807	76.777	47.120	1.00	57.32
ATOM	4294	N	SER	A	545	43.141	76.978	45.604	1.00	55.86
ATOM	4295	CA	SER	A	545	43.202	78.440	45.530	1.00	57.50
ATOM	4296	CB	SER	A	545	42.077	78.982	44.650	1.00	55.91
ATOM	4297	OG	SER	A	545	42.176	78.495	43.332	1.00	55.54
ATOM	4298	C	SER	A	545	43.074	79.083	46.902	1.00	58.62
ATOM	4299	O	SER	A	545	42.340	78.593	47.742	1.00	57.43
ATOM	4300	N	ASN	A	546	43.779	80.195	47.107	1.00	62.43
ATOM	4301	CA	ASN	A	546	43.748	80.938	48.369	1.00	63.81
ATOM	4302	CB	ASN	A	546	42.331	81.048	48.924	1.00	68.17
ATOM	4303	CG	ASN	A	546	41.477	82.058	48.205	1.00	74.32
ATOM	4304	OD1	ASN	A	546	40.381	82.367	48.688	1.00	77.91
ATOM	4305	ND2	ASN	A	546	41.931	82.577	47.068	1.00	77.22
ATOM	4306	C	ASN	A	546	44.586	80.316	49.471	1.00	62.83
ATOM	4307	O	ASN	A	546	44.842	80.960	50.485	1.00	64.71
ATOM	4308	N	SER	A	547	44.998	79.070	49.304	1.00	58.60

178/396

Figure 2A-78

ATOM	4309	CA	SER	A	547	45.769	78.438	50.360	1.00	57.80
ATOM	4310	CB	SER	A	547	45.437	76.950	50.428	1.00	53.87
ATOM	4311	OG	SER	A	547	46.130	76.332	51.491	1.00	52.30
ATOM	4312	C	SER	A	547	47.284	78.623	50.268	1.00	59.65
ATOM	4313	O	SER	A	547	47.964	77.885	49.552	1.00	61.43
ATOM	4314	N	THR	A	548	47.808	79.609	50.998	1.00	58.55
ATOM	4315	CA	THR	A	548	49.249	79.856	51.020	1.00	59.99
ATOM	4316	CB	THR	A	548	49.616	81.198	51.729	1.00	59.02
ATOM	4317	OG1	THR	A	548	48.935	81.282	52.980	1.00	59.52
ATOM	4318	CG2	THR	A	548	49.223	82.394	50.876	1.00	61.27
ATOM	4319	C	THR	A	548	49.890	78.696	51.778	1.00	59.98
ATOM	4320	O	THR	A	548	51.081	78.413	51.634	1.00	61.22
ATOM	4321	N	GLU	A	549	49.096	78.012	52.587	1.00	58.17
ATOM	4322	CA	GLU	A	549	49.625	76.878	53.316	1.00	61.31
ATOM	4323	CB	GLU	A	549	48.611	76.393	54.351	1.00	66.91
ATOM	4324	CG	GLU	A	549	49.263	76.039	55.666	1.00	75.97
ATOM	4325	CD	GLU	A	549	50.029	77.217	56.243	1.00	81.44
ATOM	4326	OE1	GLU	A	549	49.372	78.207	56.641	1.00	84.78
ATOM	4327	OE2	GLU	A	549	51.282	77.162	56.283	1.00	83.35
ATOM	4328	C	GLU	A	549	49.918	75.773	52.299	1.00	59.19
ATOM	4329	O	GLU	A	549	50.905	75.048	52.411	1.00	58.26
ATOM	4330	N	ALA	A	550	49.052	75.657	51.299	1.00	57.90
ATOM	4331	CA	ALA	A	550	49.223	74.653	50.257	1.00	57.18
ATOM	4332	CB	ALA	A	550	47.961	74.566	49.402	1.00	57.47
ATOM	4333	C	ALA	A	550	50.417	75.038	49.400	1.00	55.24
ATOM	4334	O	ALA	A	550	51.318	74.228	49.167	1.00	55.64
ATOM	4335	N	GLY	A	551	50.421	76.287	48.944	1.00	55.36
ATOM	4336	CA	GLY	A	551	51.510	76.788	48.122	1.00	53.13
ATOM	4337	C	GLY	A	551	52.866	76.729	48.808	1.00	54.98
ATOM	4338	O	GLY	A	551	53.897	76.596	48.144	1.00	55.16
ATOM	4339	N	GLN	A	552	52.884	76.827	50.134	1.00	54.52
ATOM	4340	CA	GLN	A	552	54.150	76.771	50.862	1.00	56.55
ATOM	4341	CB	GLN	A	552	53.979	77.239	52.309	1.00	56.67
ATOM	4342	CG	GLN	A	552	55.265	77.112	53.127	1.00	59.84
ATOM	4343	CD	GLN	A	552	56.387	78.008	52.606	1.00	62.69
ATOM	4344	OE1	GLN	A	552	56.257	79.236	52.599	1.00	64.78
ATOM	4345	NE2	GLN	A	552	57.491	77.397	52.164	1.00	58.95
ATOM	4346	C	GLN	A	552	54.685	75.347	50.858	1.00	56.21
ATOM	4347	O	GLN	A	552	55.854	75.118	50.541	1.00	56.72
ATOM	4348	N	LYS	A	553	53.828	74.394	51.222	1.00	56.34
ATOM	4349	CA	LYS	A	553	54.224	72.995	51.237	1.00	56.58
ATOM	4350	CB	LYS	A	553	53.065	72.100	51.697	1.00	60.67
ATOM	4351	CG	LYS	A	553	52.756	72.201	53.192	1.00	66.21
ATOM	4352	CD	LYS	A	553	51.901	71.037	53.661	1.00	69.07
ATOM	4353	CE	LYS	A	553	52.594	69.718	53.356	1.00	70.70
ATOM	4354	NZ	LYS	A	553	53.927	69.640	54.027	1.00	73.66
ATOM	4355	C	LYS	A	553	54.679	72.577	49.842	1.00	55.57
ATOM	4356	O	LYS	A	553	55.665	71.860	49.697	1.00	54.17
ATOM	4357	N	LEU	A	554	53.967	73.033	48.814	1.00	53.20
ATOM	4358	CA	LEU	A	554	54.331	72.683	47.450	1.00	52.43
ATOM	4359	CB	LEU	A	554	53.286	73.232	46.470	1.00	51.50
ATOM	4360	CG	LEU	A	554	53.454	72.972	44.968	1.00	53.28
ATOM	4361	CD1	LEU	A	554	53.645	71.498	44.670	1.00	47.15
ATOM	4362	CD2	LEU	A	554	52.222	73.482	44.260	1.00	50.83
ATOM	4363	C	LEU	A	554	55.712	73.252	47.134	1.00	50.93
ATOM	4364	O	LEU	A	554	56.600	72.544	46.644	1.00	50.89

179/396

Figure 2A-79

ATOM	4365	N	PHE	A	555	55.900	74.526	47.447	1.00	50.24
ATOM	4366	CA	PHE	A	555	57.168	75.195	47.177	1.00	52.00
ATOM	4367	CB	PHE	A	555	57.040	76.684	47.501	1.00	51.61
ATOM	4368	CG	PHE	A	555	58.264	77.484	47.173	1.00	53.57
ATOM	4369	CD1	PHE	A	555	59.302	77.612	48.099	1.00	53.41
ATOM	4370	CD2	PHE	A	555	58.382	78.119	45.937	1.00	52.74
ATOM	4371	CE1	PHE	A	555	60.435	78.366	47.798	1.00	54.79
ATOM	4372	CE2	PHE	A	555	59.514	78.875	45.625	1.00	53.07
ATOM	4373	CZ	PHE	A	555	60.541	79.000	46.558	1.00	52.19
ATOM	4374	C	PHE	A	555	58.396	74.607	47.882	1.00	52.42
ATOM	4375	O	PHE	A	555	59.497	74.671	47.352	1.00	54.72
ATOM	4376	N	ASN	A	556	58.222	74.040	49.067	1.00	54.87
ATOM	4377	CA	ASN	A	556	59.357	73.454	49.782	1.00	55.39
ATOM	4378	CB	ASN	A	556	58.918	72.915	51.150	1.00	58.35
ATOM	4379	CG	ASN	A	556	58.543	74.025	52.127	1.00	62.22
ATOM	4380	OD1	ASN	A	556	57.981	73.761	53.199	1.00	61.23
ATOM	4381	ND2	ASN	A	556	58.857	75.272	51.763	1.00	58.81
ATOM	4382	C	ASN	A	556	60.022	72.334	48.986	1.00	54.51
ATOM	4383	O	ASN	A	556	61.222	72.098	49.130	1.00	55.38
ATOM	4384	N	MET	A	557	59.257	71.618	48.163	1.00	52.28
ATOM	4385	CA	MET	A	557	59.874	70.561	47.367	1.00	48.64
ATOM	4386	CB	MET	A	557	58.952	69.347	47.259	1.00	48.27
ATOM	4387	CG	MET	A	557	57.889	69.475	46.234	1.00	56.45
ATOM	4388	SD	MET	A	557	58.406	68.958	44.578	1.00	54.50
ATOM	4389	CE	MET	A	557	56.781	68.804	43.854	1.00	49.96
ATOM	4390	C	MET	A	557	60.235	71.086	45.978	1.00	46.00
ATOM	4391	O	MET	A	557	61.193	70.626	45.358	1.00	45.42
ATOM	4392	N	LEU	A	558	59.472	72.065	45.505	1.00	46.37
ATOM	4393	CA	LEU	A	558	59.695	72.667	44.192	1.00	46.57
ATOM	4394	CB	LEU	A	558	58.602	73.716	43.944	1.00	46.34
ATOM	4395	CG	LEU	A	558	57.571	73.570	42.817	1.00	47.51
ATOM	4396	CD1	LEU	A	558	57.011	72.169	42.745	1.00	43.78
ATOM	4397	CD2	LEU	A	558	56.453	74.552	43.036	1.00	41.98
ATOM	4398	C	LEU	A	558	61.100	73.308	44.050	1.00	48.35
ATOM	4399	O	LEU	A	558	61.812	73.078	43.062	1.00	44.33
ATOM	4400	N	ARG	A	559	61.513	74.098	45.042	1.00	48.69
ATOM	4401	CA	ARG	A	559	62.819	74.757	44.966	1.00	49.92
ATOM	4402	CB	ARG	A	559	62.939	75.859	46.030	1.00	53.57
ATOM	4403	CG	ARG	A	559	63.000	75.333	47.444	1.00	59.88
ATOM	4404	CD	ARG	A	559	63.518	76.381	48.428	1.00	64.25
ATOM	4405	NE	ARG	A	559	64.171	75.702	49.543	1.00	70.97
ATOM	4406	CZ	ARG	A	559	65.433	75.270	49.534	1.00	71.88
ATOM	4407	NH1	ARG	A	559	66.207	75.462	48.473	1.00	71.23
ATOM	4408	NH2	ARG	A	559	65.910	74.599	50.574	1.00	74.39
ATOM	4409	C	ARG	A	559	63.986	73.782	45.097	1.00	46.87
ATOM	4410	O	ARG	A	559	65.123	74.132	44.824	1.00	46.94
ATOM	4411	N	LEU	A	560	63.710	72.550	45.500	1.00	45.64
ATOM	4412	CA	LEU	A	560	64.775	71.561	45.639	1.00	44.56
ATOM	4413	CB	LEU	A	560	64.241	70.334	46.388	1.00	47.34
ATOM	4414	CG	LEU	A	560	64.410	70.148	47.913	1.00	52.44
ATOM	4415	CD1	LEU	A	560	65.121	71.334	48.579	1.00	47.37
ATOM	4416	CD2	LEU	A	560	63.055	69.921	48.509	1.00	48.30
ATOM	4417	C	LEU	A	560	65.347	71.108	44.292	1.00	45.18
ATOM	4418	O	LEU	A	560	66.520	70.703	44.195	1.00	44.97
ATOM	4419	N	GLY	A	561	64.528	71.173	43.242	1.00	39.82
ATOM	4420	CA	GLY	A	561	65.005	70.682	41.972	1.00	37.98

180/396

Figure 2A-80

ATOM	4421	C	GLY	A	561	65.350	69.228	42.232	1.00	37.68
ATOM	4422	O	GLY	A	561	64.573	68.498	42.838	1.00	37.00
ATOM	4423	N	LYS	A	562	66.508	68.795	41.767	1.00	38.22
ATOM	4424	CA	LYS	A	562	66.943	67.429	42.007	1.00	43.15
ATOM	4425	CB	LYS	A	562	67.355	66.756	40.683	1.00	44.97
ATOM	4426	CG	LYS	A	562	66.795	65.348	40.521	1.00	53.55
ATOM	4427	CD	LYS	A	562	67.740	64.382	39.767	1.00	60.24
ATOM	4428	CE	LYS	A	562	68.108	64.878	38.373	1.00	62.98
ATOM	4429	NZ	LYS	A	562	68.888	66.145	38.432	1.00	59.24
ATOM	4430	C	LYS	A	562	68.148	67.426	42.993	1.00	41.99
ATOM	4431	O	LYS	A	562	68.983	66.526	42.951	1.00	41.10
ATOM	4432	N	SER	A	563	68.234	68.430	43.864	1.00	43.60
ATOM	4433	CA	SER	A	563	69.338	68.505	44.836	1.00	49.53
ATOM	4434	CB	SER	A	563	69.497	69.933	45.376	1.00	45.64
ATOM	4435	OG	SER	A	563	68.410	70.293	46.212	1.00	47.70
ATOM	4436	C	SER	A	563	69.166	67.546	46.023	1.00	51.60
ATOM	4437	O	SER	A	563	70.119	67.268	46.746	1.00	53.71
ATOM	4438	N	GLU	A	564	67.952	67.043	46.223	1.00	53.85
ATOM	4439	CA	GLU	A	564	67.682	66.120	47.317	1.00	54.21
ATOM	4440	CB	GLU	A	564	66.679	66.742	48.294	1.00	53.13
ATOM	4441	CG	GLU	A	564	67.220	67.947	49.059	1.00	58.21
ATOM	4442	CD	GLU	A	564	68.434	67.583	49.928	1.00	60.73
ATOM	4443	OE1	GLU	A	564	68.288	66.737	50.836	1.00	59.66
ATOM	4444	OE2	GLU	A	564	69.532	68.134	49.694	1.00	62.45
ATOM	4445	C	GLU	A	564	67.125	64.814	46.780	1.00	55.04
ATOM	4446	O	GLU	A	564	66.688	64.749	45.639	1.00	58.16
ATOM	4447	N	PRO	A	565	67.159	63.744	47.588	1.00	55.04
ATOM	4448	CD	PRO	A	565	67.801	63.594	48.909	1.00	54.15
ATOM	4449	CA	PRO	A	565	66.620	62.469	47.111	1.00	50.37
ATOM	4450	CB	PRO	A	565	66.829	61.535	48.309	1.00	51.99
ATOM	4451	CG	PRO	A	565	68.049	62.106	48.979	1.00	54.06
ATOM	4452	C	PRO	A	565	65.144	62.738	46.844	1.00	47.81
ATOM	4453	O	PRO	A	565	64.524	63.526	47.571	1.00	43.29
ATOM	4454	N	TRP	A	566	64.579	62.104	45.813	1.00	46.44
ATOM	4455	CA	TRP	A	566	63.168	62.328	45.493	1.00	41.89
ATOM	4456	CB	TRP	A	566	62.758	61.548	44.229	1.00	40.75
ATOM	4457	CG	TRP	A	566	62.840	60.049	44.353	1.00	31.18
ATOM	4458	CD2	TRP	A	566	61.823	59.173	44.860	1.00	27.95
ATOM	4459	CE2	TRP	A	566	62.313	57.862	44.752	1.00	33.13
ATOM	4460	CE3	TRP	A	566	60.546	59.374	45.392	1.00	33.56
ATOM	4461	CD1	TRP	A	566	63.876	59.260	43.978	1.00	30.65
ATOM	4462	NE1	TRP	A	566	63.572	57.941	44.212	1.00	36.15
ATOM	4463	CZ2	TRP	A	566	61.564	56.743	45.149	1.00	35.19
ATOM	4464	CZ3	TRP	A	566	59.798	58.260	45.792	1.00	35.35
ATOM	4465	CH2	TRP	A	566	60.315	56.963	45.663	1.00	34.58
ATOM	4466	C	TRP	A	566	62.329	61.884	46.686	1.00	42.69
ATOM	4467	O	TRP	A	566	61.262	62.444	46.962	1.00	43.12
ATOM	4468	N	THR	A	567	62.826	60.880	47.400	1.00	43.13
ATOM	4469	CA	THR	A	567	62.143	60.378	48.592	1.00	45.33
ATOM	4470	CB	THR	A	567	62.924	59.204	49.221	1.00	46.65
ATOM	4471	OG1	THR	A	567	64.281	59.606	49.462	1.00	49.15
ATOM	4472	CG2	THR	A	567	62.914	58.015	48.289	1.00	46.78
ATOM	4473	C	THR	A	567	61.976	61.476	49.655	1.00	44.76
ATOM	4474	O	THR	A	567	61.045	61.452	50.442	1.00	47.17
ATOM	4475	N	LEU	A	568	62.886	62.438	49.669	1.00	47.25
ATOM	4476	CA	LEU	A	568	62.827	63.541	50.618	1.00	47.47

181/396

Figure 2A-81

ATOM	4477	CB	LEU	A	568	64.246	64.070	50.892	1.00	49.34
ATOM	4478	CG	LEU	A	568	64.443	65.085	52.028	1.00	54.15
ATOM	4479	CD1	LEU	A	568	65.948	65.295	52.244	1.00	53.93
ATOM	4480	CD2	LEU	A	568	63.761	66.411	51.696	1.00	52.53
ATOM	4481	C	LEU	A	568	61.939	64.665	50.075	1.00	47.04
ATOM	4482	O	LEU	A	568	61.187	65.290	50.828	1.00	47.48
ATOM	4483	N	ALA	A	569	62.044	64.945	48.776	1.00	46.88
ATOM	4484	CA	ALA	A	569	61.205	65.981	48.170	1.00	44.47
ATOM	4485	CB	ALA	A	569	61.539	66.134	46.695	1.00	47.10
ATOM	4486	C	ALA	A	569	59.751	65.577	48.348	1.00	40.68
ATOM	4487	O	ALA	A	569	58.903	66.390	48.662	1.00	42.19
ATOM	4488	N	LEU	A	570	59.461	64.298	48.162	1.00	44.21
ATOM	4489	CA	LEU	A	570	58.095	63.799	48.340	1.00	43.81
ATOM	4490	CB	LEU	A	570	58.056	62.287	48.111	1.00	45.01
ATOM	4491	CG	LEU	A	570	56.879	61.609	47.412	1.00	45.39
ATOM	4492	CD1	LEU	A	570	56.851	60.162	47.865	1.00	44.64
ATOM	4493	CD2	LEU	A	570	55.577	62.293	47.721	1.00	42.63
ATOM	4494	C	LEU	A	570	57.682	64.067	49.776	1.00	45.45
ATOM	4495	O	LEU	A	570	56.632	64.665	50.052	1.00	44.73
ATOM	4496	N	GLU	A	571	58.521	63.596	50.696	1.00	48.58
ATOM	4497	CA	GLU	A	571	58.264	63.756	52.128	1.00	52.49
ATOM	4498	CB	GLU	A	571	59.447	63.238	52.958	1.00	54.90
ATOM	4499	CG	GLU	A	571	59.170	63.223	54.462	1.00	60.67
ATOM	4500	CD	GLU	A	571	60.369	62.760	55.276	1.00	62.32
ATOM	4501	OE1	GLU	A	571	61.389	63.483	55.310	1.00	62.07
ATOM	4502	OE2	GLU	A	571	60.291	61.664	55.871	1.00	63.94
ATOM	4503	C	GLU	A	571	57.990	65.204	52.488	1.00	50.29
ATOM	4504	O	GLU	A	571	57.095	65.490	53.274	1.00	50.74
ATOM	4505	N	ASN	A	572	58.754	66.123	51.908	1.00	53.37
ATOM	4506	CA	ASN	A	572	58.544	67.536	52.188	1.00	55.99
ATOM	4507	CB	ASN	A	572	59.546	68.379	51.401	1.00	60.38
ATOM	4508	CG	ASN	A	572	60.961	68.257	51.943	1.00	61.91
ATOM	4509	OD1	ASN	A	572	61.256	67.363	52.736	1.00	64.82
ATOM	4510	ND2	ASN	A	572	61.842	69.155	51.516	1.00	60.86
ATOM	4511	C	ASN	A	572	57.119	67.954	51.836	1.00	57.21
ATOM	4512	O	ASN	A	572	56.592	68.919	52.388	1.00	59.35
ATOM	4513	N	VAL	A	573	56.489	67.222	50.920	1.00	56.79
ATOM	4514	CA	VAL	A	573	55.127	67.548	50.511	1.00	54.59
ATOM	4515	CB	VAL	A	573	54.972	67.507	48.966	1.00	54.25
ATOM	4516	CG1	VAL	A	573	53.504	67.623	48.571	1.00	53.64
ATOM	4517	CG2	VAL	A	573	55.725	68.638	48.364	1.00	54.43
ATOM	4518	C	VAL	A	573	54.040	66.668	51.115	1.00	53.06
ATOM	4519	O	VAL	A	573	53.034	67.177	51.602	1.00	51.61
ATOM	4520	N	VAL	A	574	54.219	65.354	51.096	1.00	52.87
ATOM	4521	CA	VAL	A	574	53.157	64.511	51.624	1.00	53.88
ATOM	4522	CB	VAL	A	574	52.791	63.386	50.619	1.00	52.46
ATOM	4523	CG1	VAL	A	574	52.470	64.005	49.254	1.00	51.64
ATOM	4524	CG2	VAL	A	574	53.914	62.383	50.522	1.00	41.77
ATOM	4525	C	VAL	A	574	53.370	63.901	53.001	1.00	56.88
ATOM	4526	O	VAL	A	574	52.473	63.233	53.511	1.00	54.90
ATOM	4527	N	GLY	A	575	54.544	64.128	53.598	1.00	59.77
ATOM	4528	CA	GLY	A	575	54.824	63.599	54.927	1.00	59.34
ATOM	4529	C	GLY	A	575	55.190	62.125	54.977	1.00	61.11
ATOM	4530	O	GLY	A	575	55.107	61.493	56.029	1.00	63.59
ATOM	4531	N	ALA	A	576	55.598	61.574	53.842	1.00	60.01
ATOM	4532	CA	ALA	A	576	55.981	60.175	53.754	1.00	56.86

182/396

Figure 2A-82

ATOM	4533	CB	ALA	A	576	54.781	59.326	53.364	1.00	58.90
ATOM	4534	C	ALA	A	576	57.056	60.107	52.684	1.00	56.89
ATOM	4535	O	ALA	A	576	57.084	60.944	51.785	1.00	53.65
ATOM	4536	N	LYS	A	577	57.938	59.117	52.766	1.00	55.74
ATOM	4537	CA	LYS	A	577	59.018	59.026	51.798	1.00	55.69
ATOM	4538	CB	LYS	A	577	60.339	58.727	52.508	1.00	56.24
ATOM	4539	CG	LYS	A	577	60.381	57.411	53.238	1.00	60.13
ATOM	4540	CD	LYS	A	577	61.621	57.323	54.142	1.00	63.72
ATOM	4541	CE	LYS	A	577	61.628	58.427	55.202	1.00	66.52
ATOM	4542	NZ	LYS	A	577	62.704	58.241	56.224	1.00	68.71
ATOM	4543	C	LYS	A	577	58.800	58.032	50.676	1.00	54.44
ATOM	4544	O	LYS	A	577	59.716	57.754	49.898	1.00	52.19
ATOM	4545	N	ASN	A	578	57.608	57.467	50.583	1.00	52.18
ATOM	4546	CA	ASN	A	578	57.412	56.568	49.474	1.00	54.31
ATOM	4547	CB	ASN	A	578	57.564	55.113	49.892	1.00	58.26
ATOM	4548	CG	ASN	A	578	58.224	54.279	48.797	1.00	66.01
ATOM	4549	OD1	ASN	A	578	58.120	54.602	47.601	1.00	61.26
ATOM	4550	ND2	ASN	A	578	58.909	53.204	49.195	1.00	69.36
ATOM	4551	C	ASN	A	578	56.128	56.732	48.691	1.00	50.13
ATOM	4552	O	ASN	A	578	55.186	57.408	49.110	1.00	49.14
ATOM	4553	N	MET	A	579	56.137	56.126	47.515	1.00	50.25
ATOM	4554	CA	MET	A	579	55.004	56.132	46.614	1.00	50.02
ATOM	4555	CB	MET	A	579	55.414	55.484	45.287	1.00	49.33
ATOM	4556	CG	MET	A	579	54.310	55.368	44.242	1.00	52.22
ATOM	4557	SD	MET	A	579	54.932	54.711	42.653	1.00	51.74
ATOM	4558	CE	MET	A	579	55.443	53.033	43.149	1.00	50.28
ATOM	4559	C	MET	A	579	53.915	55.326	47.315	1.00	50.60
ATOM	4560	O	MET	A	579	54.152	54.217	47.794	1.00	52.21
ATOM	4561	N	ASN	A	580	52.730	55.913	47.394	1.00	50.58
ATOM	4562	CA	ASN	A	580	51.589	55.299	48.038	1.00	48.10
ATOM	4563	CB	ASN	A	580	51.358	55.979	49.385	1.00	51.47
ATOM	4564	CG	ASN	A	580	50.147	55.458	50.088	1.00	53.18
ATOM	4565	OD1	ASN	A	580	49.496	56.182	50.849	1.00	62.96
ATOM	4566	ND2	ASN	A	580	49.826	54.194	49.848	1.00	56.37
ATOM	4567	C	ASN	A	580	50.348	55.463	47.148	1.00	47.83
ATOM	4568	O	ASN	A	580	50.100	56.546	46.608	1.00	45.46
ATOM	4569	N	VAL	A	581	49.553	54.402	47.032	1.00	46.09
ATOM	4570	CA	VAL	A	581	48.366	54.425	46.193	1.00	46.92
ATOM	4571	CB	VAL	A	581	48.164	53.050	45.489	1.00	52.42
ATOM	4572	CG1	VAL	A	581	47.587	52.034	46.472	1.00	53.68
ATOM	4573	CG2	VAL	A	581	47.266	53.207	44.263	1.00	51.89
ATOM	4574	C	VAL	A	581	47.064	54.808	46.870	1.00	48.05
ATOM	4575	O	VAL	A	581	46.056	55.004	46.188	1.00	46.93
ATOM	4576	N	ARG	A	582	47.064	54.937	48.195	1.00	49.13
ATOM	4577	CA	ARG	A	582	45.824	55.273	48.902	1.00	51.27
ATOM	4578	CB	ARG	A	582	46.053	55.351	50.422	1.00	56.16
ATOM	4579	CG	ARG	A	582	45.780	54.037	51.152	1.00	66.70
ATOM	4580	CD	ARG	A	582	47.012	53.547	51.925	1.00	71.40
ATOM	4581	NE	ARG	A	582	47.419	54.501	52.957	1.00	76.75
ATOM	4582	CZ	ARG	A	582	48.581	54.449	53.605	1.00	79.43
ATOM	4583	NH1	ARG	A	582	49.454	53.483	53.329	1.00	79.02
ATOM	4584	NH2	ARG	A	582	48.876	55.368	54.521	1.00	80.90
ATOM	4585	C	ARG	A	582	45.142	56.552	48.440	1.00	47.20
ATOM	4586	O	ARG	A	582	43.917	56.616	48.357	1.00	47.10
ATOM	4587	N	PRO	A	583	45.921	57.606	48.174	1.00	46.61
ATOM	4588	CD	PRO	A	583	47.327	57.837	48.546	1.00	45.87

183/396

Figure 2A-83

ATOM	4589	CA	PRO	A	583	45.297	58.854	47.724	1.00	44.24
ATOM	4590	CB	PRO	A	583	46.475	59.809	47.644	1.00	42.67
ATOM	4591	CG	PRO	A	583	47.341	59.324	48.794	1.00	43.10
ATOM	4592	C	PRO	A	583	44.574	58.702	46.391	1.00	43.41
ATOM	4593	O	PRO	A	583	43.532	59.326	46.186	1.00	45.34
ATOM	4594	N	LEU	A	584	45.120	57.886	45.487	1.00	43.88
ATOM	4595	CA	LEU	A	584	44.477	57.678	44.191	1.00	45.06
ATOM	4596	CB	LEU	A	584	45.331	56.778	43.281	1.00	44.96
ATOM	4597	CG	LEU	A	584	44.665	56.300	41.980	1.00	52.76
ATOM	4598	CD1	LEU	A	584	45.661	56.230	40.836	1.00	55.17
ATOM	4599	CD2	LEU	A	584	44.044	54.929	42.216	1.00	55.91
ATOM	4600	C	LEU	A	584	43.133	57.031	44.489	1.00	46.21
ATOM	4601	O	LEU	A	584	42.099	57.459	43.985	1.00	44.42
ATOM	4602	N	LEU	A	585	43.157	56.022	45.353	1.00	46.35
ATOM	4603	CA	LEU	A	585	41.951	55.303	45.751	1.00	47.58
ATOM	4604	CB	LEU	A	585	42.322	54.146	46.681	1.00	47.04
ATOM	4605	CG	LEU	A	585	42.564	52.754	46.102	1.00	51.18
ATOM	4606	CD1	LEU	A	585	42.883	52.812	44.587	1.00	48.78
ATOM	4607	CD2	LEU	A	585	43.679	52.091	46.901	1.00	47.93
ATOM	4608	C	LEU	A	585	40.951	56.214	46.451	1.00	48.22
ATOM	4609	O	LEU	A	585	39.738	56.082	46.269	1.00	48.57
ATOM	4610	N	ASN	A	586	41.449	57.126	47.278	1.00	47.76
ATOM	4611	CA	ASN	A	586	40.538	58.029	47.972	1.00	49.38
ATOM	4612	CB	ASN	A	586	41.287	58.918	48.971	1.00	52.80
ATOM	4613	CG	ASN	A	586	41.807	58.147	50.177	1.00	60.73
ATOM	4614	OD1	ASN	A	586	42.765	58.576	50.839	1.00	64.42
ATOM	4615	ND2	ASN	A	586	41.172	57.019	50.485	1.00	58.51
ATOM	4616	C	ASN	A	586	39.839	58.910	46.953	1.00	44.26
ATOM	4617	O	ASN	A	586	38.664	59.212	47.094	1.00	46.68
ATOM	4618	N	TYR	A	587	40.576	59.332	45.934	1.00	45.78
ATOM	4619	CA	TYR	A	587	40.029	60.201	44.888	1.00	45.37
ATOM	4620	CB	TYR	A	587	41.097	60.485	43.824	1.00	45.28
ATOM	4621	CG	TYR	A	587	40.690	61.485	42.764	1.00	46.04
ATOM	4622	CD1	TYR	A	587	40.838	62.855	42.973	1.00	45.91
ATOM	4623	CE1	TYR	A	587	40.488	63.768	41.994	1.00	43.39
ATOM	4624	CD2	TYR	A	587	40.171	61.060	41.536	1.00	46.34
ATOM	4625	CE2	TYR	A	587	39.815	61.970	40.550	1.00	42.92
ATOM	4626	CZ	TYR	A	587	39.976	63.318	40.786	1.00	44.29
ATOM	4627	OH	TYR	A	587	39.625	64.219	39.811	1.00	42.20
ATOM	4628	C	TYR	A	587	38.841	59.530	44.225	1.00	45.65
ATOM	4629	O	TYR	A	587	37.780	60.142	44.048	1.00	44.21
ATOM	4630	N	PHE	A	588	39.023	58.255	43.898	1.00	45.38
ATOM	4631	CA	PHE	A	588	38.007	57.478	43.203	1.00	46.08
ATOM	4632	CB	PHE	A	588	38.693	56.520	42.223	1.00	43.69
ATOM	4633	CG	PHE	A	588	39.277	57.203	41.023	1.00	40.01
ATOM	4634	CD1	PHE	A	588	40.654	57.304	40.857	1.00	38.63
ATOM	4635	CD2	PHE	A	588	38.435	57.758	40.048	1.00	42.25
ATOM	4636	CE1	PHE	A	588	41.197	57.950	39.734	1.00	42.36
ATOM	4637	CE2	PHE	A	588	38.960	58.406	38.922	1.00	37.58
ATOM	4638	CZ	PHE	A	588	40.339	58.505	38.758	1.00	38.51
ATOM	4639	C	PHE	A	588	37.008	56.704	44.052	1.00	48.55
ATOM	4640	O	PHE	A	588	36.131	56.019	43.506	1.00	46.84
ATOM	4641	N	GLU	A	589	37.118	56.812	45.374	1.00	49.53
ATOM	4642	CA	GLU	A	589	36.198	56.097	46.256	1.00	51.28
ATOM	4643	CB	GLU	A	589	36.451	56.479	47.713	1.00	54.01
ATOM	4644	CG	GLU	A	589	37.507	55.604	48.357	1.00	63.13

184/396

Figure 2A-84

ATOM	4645	CD	GLU	A	589	37.054	54.152	48.504	1.00	68.84
ATOM	4646	OE1	GLU	A	589	37.852	53.236	48.191	1.00	69.12
ATOM	4647	OE2	GLU	A	589	35.902	53.926	48.940	1.00	70.57
ATOM	4648	C	GLU	A	589	34.707	56.250	45.934	1.00	50.46
ATOM	4649	O	GLU	A	589	33.962	55.273	45.980	1.00	48.29
ATOM	4650	N	PRO	A	590	34.246	57.475	45.630	1.00	49.92
ATOM	4651	CD	PRO	A	590	34.920	58.788	45.707	1.00	47.39
ATOM	4652	CA	PRO	A	590	32.818	57.626	45.317	1.00	47.15
ATOM	4653	CB	PRO	A	590	32.686	59.114	45.029	1.00	46.12
ATOM	4654	CG	PRO	A	590	33.765	59.727	45.927	1.00	47.18
ATOM	4655	C	PRO	A	590	32.398	56.760	44.122	1.00	48.65
ATOM	4656	O	PRO	A	590	31.316	56.168	44.127	1.00	47.87
ATOM	4657	N	LEU	A	591	33.258	56.696	43.105	1.00	47.98
ATOM	4658	CA	LEU	A	591	32.988	55.899	41.914	1.00	47.79
ATOM	4659	CB	LEU	A	591	33.959	56.269	40.786	1.00	44.01
ATOM	4660	CG	LEU	A	591	33.874	55.369	39.542	1.00	45.12
ATOM	4661	CD1	LEU	A	591	32.564	55.624	38.815	1.00	38.33
ATOM	4662	CD2	LEU	A	591	35.033	55.632	38.601	1.00	37.50
ATOM	4663	C	LEU	A	591	33.144	54.415	42.241	1.00	50.76
ATOM	4664	O	LEU	A	591	32.427	53.568	41.707	1.00	52.49
ATOM	4665	N	PHE	A	592	34.073	54.109	43.137	1.00	51.95
ATOM	4666	CA	PHE	A	592	34.338	52.734	43.507	1.00	53.28
ATOM	4667	CB	PHE	A	592	35.570	52.662	44.400	1.00	52.54
ATOM	4668	CG	PHE	A	592	35.961	51.268	44.780	1.00	50.38
ATOM	4669	CD1	PHE	A	592	36.040	50.271	43.822	1.00	53.37
ATOM	4670	CD2	PHE	A	592	36.284	50.958	46.091	1.00	52.53
ATOM	4671	CE1	PHE	A	592	36.439	48.980	44.164	1.00	54.27
ATOM	4672	CE2	PHE	A	592	36.686	49.673	46.444	1.00	52.14
ATOM	4673	CZ	PHE	A	592	36.763	48.681	45.476	1.00	52.56
ATOM	4674	C	PHE	A	592	33.163	52.064	44.195	1.00	56.54
ATOM	4675	O	PHE	A	592	32.907	50.875	43.981	1.00	57.17
ATOM	4676	N	THR	A	593	32.439	52.817	45.012	1.00	57.17
ATOM	4677	CA	THR	A	593	31.295	52.253	45.721	1.00	60.46
ATOM	4678	CB	THR	A	593	30.923	53.129	46.927	1.00	62.02
ATOM	4679	OG1	THR	A	593	30.623	54.456	46.477	1.00	66.57
ATOM	4680	CG2	THR	A	593	32.092	53.187	47.904	1.00	60.33
ATOM	4681	C	THR	A	593	30.098	52.106	44.781	1.00	58.90
ATOM	4682	O	THR	A	593	29.303	51.177	44.903	1.00	59.33
ATOM	4683	N	TRP	A	594	29.988	53.026	43.835	1.00	57.46
ATOM	4684	CA	TRP	A	594	28.920	52.997	42.847	1.00	57.16
ATOM	4685	CB	TRP	A	594	28.961	54.272	42.023	1.00	52.08
ATOM	4686	CG	TRP	A	594	27.896	54.361	40.987	1.00	52.54
ATOM	4687	CD2	TRP	A	594	28.049	54.154	39.578	1.00	50.71
ATOM	4688	CE2	TRP	A	594	26.806	54.453	38.976	1.00	52.24
ATOM	4689	CE3	TRP	A	594	29.115	53.752	38.766	1.00	50.13
ATOM	4690	CD1	TRP	A	594	26.606	54.750	41.179	1.00	52.23
ATOM	4691	NE1	TRP	A	594	25.945	54.814	39.978	1.00	50.86
ATOM	4692	CZ2	TRP	A	594	26.596	54.365	37.594	1.00	50.38
ATOM	4693	CZ3	TRP	A	594	28.910	53.665	37.392	1.00	54.51
ATOM	4694	CH2	TRP	A	594	27.654	53.974	36.819	1.00	53.96
ATOM	4695	C	TRP	A	594	29.147	51.804	41.919	1.00	58.49
ATOM	4696	O	TRP	A	594	28.218	51.072	41.584	1.00	60.05
ATOM	4697	N	LEU	A	595	30.398	51.630	41.502	1.00	57.96
ATOM	4698	CA	LEU	A	595	30.775	50.542	40.611	1.00	57.53
ATOM	4699	CB	LEU	A	595	32.284	50.606	40.343	1.00	54.29
ATOM	4700	CG	LEU	A	595	32.791	51.009	38.948	1.00	57.14

185/396

Figure 2A-85

ATOM	4701	CD1	LEU	A	595	31.810	51.917	38.254	1.00	56.96
ATOM	4702	CD2	LEU	A	595	34.156	51.688	39.074	1.00	51.73
ATOM	4703	C	LEU	A	595	30.378	49.189	41.212	1.00	57.95
ATOM	4704	O	LEU	A	595	29.684	48.399	40.568	1.00	57.83
ATOM	4705	N	LYS	A	596	30.814	48.930	42.443	1.00	58.13
ATOM	4706	CA	LYS	A	596	30.488	47.684	43.132	1.00	57.57
ATOM	4707	CB	LYS	A	596	30.937	47.759	44.591	1.00	57.18
ATOM	4708	CG	LYS	A	596	32.427	47.490	44.784	1.00	60.25
ATOM	4709	CD	LYS	A	596	33.051	48.341	45.897	1.00	63.54
ATOM	4710	CE	LYS	A	596	32.370	48.154	47.246	1.00	67.10
ATOM	4711	NZ	LYS	A	596	33.223	48.659	48.373	1.00	69.14
ATOM	4712	C	LYS	A	596	28.994	47.392	43.060	1.00	59.03
ATOM	4713	O	LYS	A	596	28.593	46.280	42.715	1.00	58.21
ATOM	4714	N	ASP	A	597	28.176	48.397	43.370	1.00	59.20
ATOM	4715	CA	ASP	A	597	26.720	48.254	43.332	1.00	62.14
ATOM	4716	CB	ASP	A	597	26.043	49.522	43.876	1.00	64.03
ATOM	4717	CG	ASP	A	597	24.527	49.394	43.945	1.00	67.03
ATOM	4718	OD1	ASP	A	597	24.033	48.516	44.689	1.00	70.04
ATOM	4719	OD2	ASP	A	597	23.826	50.170	43.254	1.00	68.03
ATOM	4720	C	ASP	A	597	26.225	47.976	41.905	1.00	61.26
ATOM	4721	O	ASP	A	597	25.277	47.213	41.706	1.00	60.40
ATOM	4722	N	GLN	A	598	26.860	48.600	40.918	1.00	59.75
ATOM	4723	CA	GLN	A	598	26.487	48.378	39.525	1.00	59.61
ATOM	4724	CB	GLN	A	598	27.206	49.366	38.604	1.00	60.16
ATOM	4725	CG	GLN	A	598	26.678	50.802	38.639	1.00	63.30
ATOM	4726	CD	GLN	A	598	25.275	50.934	38.062	1.00	63.27
ATOM	4727	OE1	GLN	A	598	24.984	50.418	36.983	1.00	62.17
ATOM	4728	NE2	GLN	A	598	24.406	51.636	38.777	1.00	62.34
ATOM	4729	C	GLN	A	598	26.857	46.958	39.108	1.00	59.26
ATOM	4730	O	GLN	A	598	26.175	46.346	38.295	1.00	59.93
ATOM	4731	N	ASN	A	599	27.945	46.440	39.668	1.00	58.92
ATOM	4732	CA	ASN	A	599	28.421	45.098	39.350	1.00	58.22
ATOM	4733	CB	ASN	A	599	29.948	45.051	39.461	1.00	55.17
ATOM	4734	CG	ASN	A	599	30.648	45.944	38.452	1.00	52.50
ATOM	4735	OD1	ASN	A	599	31.861	46.140	38.532	1.00	53.93
ATOM	4736	ND2	ASN	A	599	29.901	46.474	37.496	1.00	43.55
ATOM	4737	C	ASN	A	599	27.832	44.031	40.283	1.00	60.74
ATOM	4738	O	ASN	A	599	28.310	42.893	40.311	1.00	60.09
ATOM	4739	N	LYS	A	600	26.805	44.399	41.040	1.00	62.77
ATOM	4740	CA	LYS	A	600	26.177	43.490	42.002	1.00	67.03
ATOM	4741	CB	LYS	A	600	24.905	44.136	42.571	1.00	71.74
ATOM	4742	CG	LYS	A	600	24.336	43.466	43.822	1.00	76.50
ATOM	4743	CD	LYS	A	600	25.217	43.702	45.055	1.00	80.04
ATOM	4744	CE	LYS	A	600	24.588	43.111	46.322	1.00	79.74
ATOM	4745	NZ	LYS	A	600	25.368	43.430	47.558	1.00	79.97
ATOM	4746	C	LYS	A	600	25.831	42.131	41.401	1.00	68.01
ATOM	4747	O	LYS	A	600	25.981	41.093	42.047	1.00	67.21
ATOM	4748	N	ASN	A	601	25.381	42.142	40.154	1.00	68.65
ATOM	4749	CA	ASN	A	601	24.993	40.912	39.478	1.00	70.37
ATOM	4750	CB	ASN	A	601	23.602	41.103	38.884	1.00	73.06
ATOM	4751	CG	ASN	A	601	23.571	42.217	37.854	1.00	76.89
ATOM	4752	OD1	ASN	A	601	24.313	43.209	37.969	1.00	75.82
ATOM	4753	ND2	ASN	A	601	22.711	42.071	36.844	1.00	75.83
ATOM	4754	C	ASN	A	601	25.961	40.478	38.371	1.00	69.54
ATOM	4755	O	ASN	A	601	25.781	39.413	37.769	1.00	72.30
ATOM	4756	N	SER	A	602	26.981	41.290	38.096	1.00	66.45

186/396

Figure 2A-86

ATOM	4757	CA	SER A 602	27.944	40.962	37.044	1.00	61.50
ATOM	4758	CB	SER A 602	28.523	42.245	36.438	1.00	60.16
ATOM	4759	OG	SER A 602	27.548	42.977	35.720	1.00	58.95
ATOM	4760	C	SER A 602	29.098	40.094	37.525	1.00	59.38
ATOM	4761	O	SER A 602	29.283	39.883	38.719	1.00	59.15
ATOM	4762	N	PHE A 603	29.864	39.575	36.575	1.00	57.78
ATOM	4763	CA	PHE A 603	31.037	38.786	36.907	1.00	58.68
ATOM	4764	CB	PHE A 603	31.346	37.768	35.800	1.00	57.85
ATOM	4765	CG	PHE A 603	32.512	36.849	36.112	1.00	56.33
ATOM	4766	CD1	PHE A 603	33.805	37.176	35.712	1.00	55.28
ATOM	4767	CD2	PHE A 603	32.312	35.665	36.811	1.00	56.11
ATOM	4768	CE1	PHE A 603	34.886	36.338	36.003	1.00	52.11
ATOM	4769	CE2	PHE A 603	33.382	34.818	37.110	1.00	56.88
ATOM	4770	CZ	PHE A 603	34.675	35.159	36.703	1.00	56.95
ATOM	4771	C	PHE A 603	32.153	39.825	37.008	1.00	58.44
ATOM	4772	O	PHE A 603	32.341	40.627	36.093	1.00	58.72
ATOM	4773	N	VAL A 604	32.854	39.844	38.136	1.00	57.25
ATOM	4774	CA	VAL A 604	33.944	40.784	38.332	1.00	56.73
ATOM	4775	CB	VAL A 604	33.900	41.417	39.741	1.00	57.30
ATOM	4776	CG1	VAL A 604	34.982	42.492	39.860	1.00	54.98
ATOM	4777	CG2	VAL A 604	32.524	42.012	39.996	1.00	56.32
ATOM	4778	C	VAL A 604	35.262	40.037	38.156	1.00	57.53
ATOM	4779	O	VAL A 604	35.574	39.111	38.916	1.00	57.87
ATOM	4780	N	GLY A 605	36.036	40.440	37.151	1.00	54.02
ATOM	4781	CA	GLY A 605	37.294	39.773	36.890	1.00	50.87
ATOM	4782	C	GLY A 605	37.199	39.135	35.521	1.00	49.73
ATOM	4783	O	GLY A 605	36.263	39.400	34.780	1.00	47.68
ATOM	4784	N	TRP A 606	38.133	38.265	35.177	1.00	48.94
ATOM	4785	CA	TRP A 606	38.081	37.682	33.854	1.00	50.87
ATOM	4786	CB	TRP A 606	38.712	38.663	32.858	1.00	50.59
ATOM	4787	CG	TRP A 606	40.097	39.108	33.277	1.00	47.95
ATOM	4788	CD2	TRP A 606	40.438	40.310	33.974	1.00	44.28
ATOM	4789	CE2	TRP A 606	41.833	40.284	34.192	1.00	45.33
ATOM	4790	CE3	TRP A 606	39.701	41.408	34.433	1.00	44.11
ATOM	4791	CD1	TRP A 606	41.270	38.420	33.105	1.00	48.38
ATOM	4792	NE1	TRP A 606	42.313	39.119	33.650	1.00	44.84
ATOM	4793	CZ2	TRP A 606	42.513	41.321	34.852	1.00	42.26
ATOM	4794	CZ3	TRP A 606	40.377	42.440	35.088	1.00	43.39
ATOM	4795	CH2	TRP A 606	41.769	42.386	35.290	1.00	38.90
ATOM	4796	C	TRP A 606	38.762	36.346	33.732	1.00	51.53
ATOM	4797	O	TRP A 606	39.615	35.988	34.539	1.00	49.58
ATOM	4798	N	SER A 607	38.374	35.621	32.690	1.00	55.10
ATOM	4799	CA	SER A 607	38.941	34.313	32.373	1.00	56.60
ATOM	4800	CB	SER A 607	37.844	33.396	31.818	1.00	60.53
ATOM	4801	OG	SER A 607	38.372	32.426	30.922	1.00	64.92
ATOM	4802	C	SER A 607	39.983	34.571	31.299	1.00	53.71
ATOM	4803	O	SER A 607	39.723	35.338	30.380	1.00	54.31
ATOM	4804	N	THR A 608	41.152	33.946	31.393	1.00	53.87
ATOM	4805	CA	THR A 608	42.174	34.177	30.378	1.00	57.27
ATOM	4806	CB	THR A 608	43.588	34.100	30.975	1.00	58.91
ATOM	4807	OG1	THR A 608	43.870	32.755	31.391	1.00	56.58
ATOM	4808	CG2	THR A 608	43.707	35.051	32.157	1.00	57.45
ATOM	4809	C	THR A 608	42.097	33.208	29.196	1.00	59.76
ATOM	4810	O	THR A 608	42.919	33.267	28.283	1.00	60.37
ATOM	4811	N	ASP A 609	41.094	32.334	29.210	1.00	62.01
ATOM	4812	CA	ASP A 609	40.919	31.335	28.158	1.00	61.76

187/396

Figure 2A-87

ATOM	4813	CB	ASP	A	609	40.150	30.126	28.697	1.00	65.47
ATOM	4814	CG	ASP	A	609	40.894	29.403	29.797	1.00	70.01
ATOM	4815	OD1	ASP	A	609	40.299	28.482	30.394	1.00	75.46
ATOM	4816	OD2	ASP	A	609	42.067	29.746	30.062	1.00	72.63
ATOM	4817	C	ASP	A	609	40.178	31.862	26.949	1.00	59.77
ATOM	4818	O	ASP	A	609	40.555	31.591	25.811	1.00	61.60
ATOM	4819	N	TRP	A	610	39.116	32.612	27.195	1.00	57.27
ATOM	4820	CA	TRP	A	610	38.315	33.136	26.107	1.00	57.54
ATOM	4821	CB	TRP	A	610	37.116	33.900	26.664	1.00	54.91
ATOM	4822	CG	TRP	A	610	36.186	34.361	25.587	1.00	55.07
ATOM	4823	CD2	TRP	A	610	36.175	35.651	24.953	1.00	52.06
ATOM	4824	CE2	TRP	A	610	35.148	35.629	23.984	1.00	51.22
ATOM	4825	CE3	TRP	A	610	36.933	36.821	25.110	1.00	52.70
ATOM	4826	CD1	TRP	A	610	35.198	33.632	24.991	1.00	52.60
ATOM	4827	NE1	TRP	A	610	34.571	34.387	24.028	1.00	52.31
ATOM	4828	CZ2	TRP	A	610	34.854	36.735	23.173	1.00	49.53
ATOM	4829	CZ3	TRP	A	610	36.641	37.928	24.299	1.00	47.96
ATOM	4830	CH2	TRP	A	610	35.611	37.872	23.348	1.00	51.15
ATOM	4831	C	TRP	A	610	39.070	34.035	25.131	1.00	59.20
ATOM	4832	O	TRP	A	610	39.989	34.775	25.510	1.00	58.64
ATOM	4833	N	SER	A	611	38.682	33.948	23.862	1.00	58.96
ATOM	4834	CA	SER	A	611	39.270	34.773	22.818	1.00	60.97
ATOM	4835	CB	SER	A	611	40.571	34.158	22.280	1.00	59.72
ATOM	4836	OG	SER	A	611	40.349	32.913	21.654	1.00	59.31
ATOM	4837	C	SER	A	611	38.233	34.899	21.712	1.00	61.50
ATOM	4838	O	SER	A	611	37.384	34.023	21.548	1.00	62.46
ATOM	4839	N	PRO	A	612	38.278	36.001	20.947	1.00	61.55
ATOM	4840	CD	PRO	A	612	39.221	37.125	21.071	1.00	60.63
ATOM	4841	CA	PRO	A	612	37.333	36.245	19.855	1.00	60.79
ATOM	4842	CB	PRO	A	612	37.844	37.554	19.247	1.00	56.76
ATOM	4843	CG	PRO	A	612	38.459	38.245	20.412	1.00	59.03
ATOM	4844	C	PRO	A	612	37.291	35.118	18.825	1.00	61.09
ATOM	4845	O	PRO	A	612	36.255	34.862	18.209	1.00	59.36
ATOM	4846	N	TYR	A	613	38.420	34.442	18.653	1.00	61.95
ATOM	4847	CA	TYR	A	613	38.528	33.373	17.669	1.00	64.81
ATOM	4848	CB	TYR	A	613	39.844	33.552	16.901	1.00	60.73
ATOM	4849	CG	TYR	A	613	41.068	33.594	17.795	1.00	57.52
ATOM	4850	CD1	TYR	A	613	41.675	32.421	18.235	1.00	54.65
ATOM	4851	CE1	TYR	A	613	42.776	32.455	19.089	1.00	54.95
ATOM	4852	CD2	TYR	A	613	41.598	34.813	18.235	1.00	56.67
ATOM	4853	CE2	TYR	A	613	42.699	34.854	19.094	1.00	50.52
ATOM	4854	CZ	TYR	A	613	43.278	33.675	19.514	1.00	53.33
ATOM	4855	OH	TYR	A	613	44.363	33.704	20.359	1.00	59.27
ATOM	4856	C	TYR	A	613	38.445	31.953	18.236	1.00	68.07
ATOM	4857	O	TYR	A	613	38.587	30.980	17.498	1.00	66.41
ATOM	4858	N	ALA	A	614	38.212	31.832	19.538	1.00	71.88
ATOM	4859	CA	ALA	A	614	38.139	30.518	20.166	1.00	77.39
ATOM	4860	CB	ALA	A	614	37.862	30.665	21.656	1.00	77.57
ATOM	4861	C	ALA	A	614	37.072	29.638	19.520	1.00	81.34
ATOM	4862	O	ALA	A	614	37.177	28.408	19.535	1.00	80.73
ATOM	4863	N	ASP	A	615	36.050	30.273	18.949	1.00	85.04
ATOM	4864	CA	ASP	A	615	34.963	29.547	18.302	1.00	88.97
ATOM	4865	CB	ASP	A	615	33.613	30.080	18.805	1.00	90.10
ATOM	4866	CG	ASP	A	615	33.436	31.567	18.552	1.00	92.73
ATOM	4867	OD1	ASP	A	615	33.122	31.951	17.402	1.00	93.72
ATOM	4868	OD2	ASP	A	615	33.620	32.357	19.504	1.00	95.16

188/396

Figure 2A-88

ATOM	4869	C	ASP	A	615	35.026	29.596	16.769	1.00	90.79
ATOM	4870	O	ASP	A	615	34.341	30.393	16.128	1.00	90.99
ATOM	4871	N	GLN	A	616	35.861	28.727	16.203	1.00	91.81
ATOM	4872	CA	GLN	A	616	36.062	28.594	14.757	1.00	92.70
ATOM	4873	CB	GLN	A	616	36.069	29.956	14.053	1.00	93.73
ATOM	4874	CG	GLN	A	616	34.702	30.364	13.521	1.00	96.06
ATOM	4875	CD	GLN	A	616	34.732	31.664	12.735	1.00	98.38
ATOM	4876	OE1	GLN	A	616	33.680	32.218	12.387	1.00	98.74
ATOM	4877	NE2	GLN	A	616	35.940	32.155	12.441	1.00	96.89
ATOM	4878	C	GLN	A	616	37.384	27.898	14.513	1.00	91.80
ATOM	4879	O	GLN	A	616	37.933	27.939	13.415	1.00	92.87
ATOM	4880	N	SER	A	617	37.885	27.239	15.547	1.00	90.46
ATOM	4881	CA	SER	A	617	39.159	26.561	15.443	1.00	90.18
ATOM	4882	CB	SER	A	617	40.115	27.115	16.502	1.00	89.59
ATOM	4883	OG	SER	A	617	40.202	28.524	16.418	1.00	88.63
ATOM	4884	C	SER	A	617	39.092	25.045	15.574	1.00	89.84
ATOM	4885	O	SER	A	617	38.256	24.499	16.293	1.00	90.88
ATOM	4886	N	ILE	A	618	39.987	24.377	14.855	1.00	89.01
ATOM	4887	CA	ILE	A	618	40.102	22.931	14.902	1.00	87.97
ATOM	4888	CB	ILE	A	618	40.181	22.311	13.499	1.00	87.12
ATOM	4889	CG2	ILE	A	618	40.451	20.821	13.623	1.00	85.76
ATOM	4890	CG1	ILE	A	618	38.882	22.563	12.728	1.00	83.52
ATOM	4891	CD1	ILE	A	618	38.626	24.008	12.379	1.00	83.10
ATOM	4892	C	ILE	A	618	41.426	22.702	15.615	1.00	89.10
ATOM	4893	O	ILE	A	618	42.422	23.344	15.286	1.00	89.43
ATOM	4894	N	LYS	A	619	41.446	21.802	16.591	1.00	91.10
ATOM	4895	CA	LYS	A	619	42.669	21.541	17.345	1.00	93.87
ATOM	4896	CB	LYS	A	619	42.328	21.339	18.827	1.00	94.47
ATOM	4897	CG	LYS	A	619	42.063	22.635	19.583	1.00	96.04
ATOM	4898	CD	LYS	A	619	41.465	22.377	20.958	1.00	96.93
ATOM	4899	CE	LYS	A	619	40.025	21.875	20.853	1.00	98.03
ATOM	4900	NZ	LYS	A	619	39.126	22.856	20.169	1.00	98.46
ATOM	4901	C	LYS	A	619	43.511	20.367	16.840	1.00	95.48
ATOM	4902	O	LYS	A	619	43.020	19.497	16.120	1.00	95.02
ATOM	4903	N	VAL	A	620	44.788	20.381	17.229	1.00	96.40
ATOM	4904	CA	VAL	A	620	45.785	19.362	16.880	1.00	98.19
ATOM	4905	CB	VAL	A	620	46.271	19.524	15.421	1.00	98.00
ATOM	4906	CG1	VAL	A	620	45.174	19.141	14.450	1.00	99.08
ATOM	4907	CG2	VAL	A	620	46.688	20.954	15.176	1.00	98.95
ATOM	4908	C	VAL	A	620	46.986	19.559	17.822	1.00	99.47
ATOM	4909	O	VAL	A	620	47.017	20.538	18.571	1.00	100.34
ATOM	4910	N	ALA	A	621	47.972	18.660	17.799	1.00	100.68
ATOM	4911	CA	ALA	A	621	49.123	18.832	18.690	1.00	101.62
ATOM	4912	CB	ALA	A	621	48.830	18.167	20.039	1.00	102.61
ATOM	4913	C	ALA	A	621	50.525	18.416	18.193	1.00	101.66
ATOM	4914	O	ALA	A	621	50.751	18.154	17.010	1.00	101.67
ATOM	4915	N	ALA	A	622	51.446	18.387	19.156	1.00	101.70
ATOM	4916	CA	ALA	A	622	52.883	18.079	19.046	1.00	101.61
ATOM	4917	CB	ALA	A	622	53.406	18.314	17.635	1.00	101.41
ATOM	4918	C	ALA	A	622	53.311	19.206	19.971	1.00	103.05
ATOM	4919	O	ALA	A	622	53.255	19.064	21.191	1.00	104.24
ATOM	4920	N	ALA	A	623	53.712	20.340	19.413	1.00	103.20
ATOM	4921	CA	ALA	A	623	54.006	21.459	20.286	1.00	102.06
ATOM	4922	CB	ALA	A	623	55.203	22.274	19.774	1.00	102.99
ATOM	4923	C	ALA	A	623	52.712	22.280	20.274	1.00	101.29
ATOM	4924	O	ALA	A	623	52.737	23.501	20.291	1.00	101.55

189/396

Figure 2A-89

ATOM	4925	N	ALA	A	624	51.583	21.569	20.213	1.00	100.54
ATOM	4926	CA	ALA	A	624	50.232	22.162	20.208	1.00	100.08
ATOM	4927	CB	ALA	A	624	50.003	22.957	21.496	1.00	100.12
ATOM	4928	C	ALA	A	624	49.902	23.048	18.996	1.00	99.33
ATOM	4929	O	ALA	A	624	50.788	23.683	18.421	1.00	100.78
ATOM	4930	N	ALA	A	625	48.622	23.087	18.612	1.00	97.51
ATOM	4931	CA	ALA	A	625	48.181	23.896	17.472	1.00	95.84
ATOM	4932	CB	ALA	A	625	48.840	23.386	16.190	1.00	95.18
ATOM	4933	C	ALA	A	625	46.663	23.957	17.279	1.00	94.43
ATOM	4934	O	ALA	A	625	45.948	22.994	17.549	1.00	95.16
ATOM	4935	N	ALA	A	626	46.196	25.104	16.789	1.00	92.11
ATOM	4936	CA	ALA	A	626	44.780	25.356	16.517	1.00	87.68
ATOM	4937	CB	ALA	A	626	44.110	25.959	17.746	1.00	87.71
ATOM	4938	C	ALA	A	626	44.744	26.344	15.355	1.00	84.69
ATOM	4939	O	ALA	A	626	45.712	27.076	15.159	1.00	84.16
ATOM	4940	N	ALA	A	804	43.646	26.384	14.597	1.00	80.65
ATOM	4941	CA	ALA	A	804	43.580	27.297	13.454	1.00	78.03
ATOM	4942	CB	ALA	A	804	44.324	26.671	12.275	1.00	78.81
ATOM	4943	C	ALA	A	804	42.194	27.781	12.986	1.00	75.92
ATOM	4944	O	ALA	A	804	41.161	27.279	13.421	1.00	76.97
ATOM	4945	N	ALA	A	805	42.203	28.764	12.082	1.00	72.34
ATOM	4946	CA	ALA	A	805	40.993	29.354	11.498	1.00	69.05
ATOM	4947	CB	ALA	A	805	40.476	30.491	12.386	1.00	71.01
ATOM	4948	C	ALA	A	805	41.358	29.886	10.108	1.00	67.73
ATOM	4949	O	ALA	A	805	42.495	29.720	9.675	1.00	67.46
ATOM	4950	N	ALA	A	806	40.419	30.531	9.415	1.00	65.98
ATOM	4951	CA	ALA	A	806	40.704	31.046	8.074	1.00	67.07
ATOM	4952	CB	ALA	A	806	40.466	29.933	7.032	1.00	66.35
ATOM	4953	C	ALA	A	806	39.935	32.306	7.672	1.00	66.61
ATOM	4954	O	ALA	A	806	38.878	32.592	8.208	1.00	68.40
ATOM	4955	N	ALA	A	807	40.480	33.042	6.707	1.00	67.05
ATOM	4956	CA	ALA	A	807	39.883	34.276	6.205	1.00	70.43
ATOM	4957	CB	ALA	A	807	40.362	35.458	7.056	1.00	72.36
ATOM	4958	C	ALA	A	807	40.394	34.406	4.767	1.00	73.81
ATOM	4959	O	ALA	A	807	40.848	33.411	4.205	1.00	75.80
ATOM	4960	N	ALA	A	808	40.343	35.601	4.169	1.00	74.80
ATOM	4961	CA	ALA	A	808	40.852	35.777	2.798	1.00	77.27
ATOM	4962	CB	ALA	A	808	39.964	35.032	1.812	1.00	77.14
ATOM	4963	C	ALA	A	808	40.989	37.236	2.362	1.00	78.66
ATOM	4964	O	ALA	A	808	40.000	37.864	1.987	1.00	79.35
ATOM	4965	N	ALA	A	809	42.222	37.749	2.388	1.00	79.67
ATOM	4966	CA	ALA	A	809	42.549	39.137	2.020	1.00	81.12
ATOM	4967	CB	ALA	A	809	43.091	39.195	0.602	1.00	81.30
ATOM	4968	C	ALA	A	809	41.359	40.078	2.157	1.00	82.53
ATOM	4969	O	ALA	A	809	40.634	40.312	1.185	1.00	83.33
ATOM	4970	N	ALA	A	810	41.187	40.611	3.370	1.00	81.21
ATOM	4971	CA	ALA	A	810	40.095	41.511	3.747	1.00	81.12
ATOM	4972	CB	ALA	A	810	39.421	42.133	2.514	1.00	82.74
ATOM	4973	C	ALA	A	810	39.078	40.702	4.545	1.00	81.79
ATOM	4974	O	ALA	A	810	39.425	39.692	5.167	1.00	80.11
ATOM	4975	N	ALA	A	811	39.852	40.806	7.281	1.00	91.92
ATOM	4976	CA	ALA	A	811	40.322	39.589	7.919	1.00	91.97
ATOM	4977	CB	ALA	A	811	41.797	39.710	8.251	1.00	91.26
ATOM	4978	C	ALA	A	811	39.519	39.348	9.192	1.00	92.37
ATOM	4979	O	ALA	A	811	40.095	39.012	10.227	1.00	91.74
ATOM	4980	N	ALA	A	812	38.193	39.502	9.114	1.00	93.62

190/396

Figure 2A-90

ATOM	4981	CA	ALA	A	812	37.332	39.338	10.284	1.00	93.73
ATOM	4982	CB	ALA	A	812	36.343	40.465	10.329	1.00	91.75
ATOM	4983	C	ALA	A	812	36.594	38.021	10.486	1.00	94.19
ATOM	4984	O	ALA	A	812	35.850	37.889	11.454	1.00	95.04
ATOM	4985	N	ALA	A	813	36.778	37.072	9.574	1.00	94.47
ATOM	4986	CA	ALA	A	813	36.174	35.748	9.685	1.00	93.48
ATOM	4987	CB	ALA	A	813	34.842	35.808	10.437	1.00	94.97
ATOM	4988	C	ALA	A	813	35.982	35.058	8.353	1.00	93.19
ATOM	4989	O	ALA	A	813	36.458	35.540	7.331	1.00	92.38
ATOM	4990	N	ALA	A	814	35.294	33.915	8.402	1.00	94.19
ATOM	4991	CA	ALA	A	814	34.985	33.059	7.251	1.00	94.75
ATOM	4992	CB	ALA	A	814	36.243	32.758	6.453	1.00	94.96
ATOM	4993	C	ALA	A	814	34.380	31.759	7.774	1.00	95.58
ATOM	4994	O	ALA	A	814	35.115	30.871	8.222	1.00	94.98
ATOM	4995	N	ALA	A	816	33.048	31.671	7.696	1.00	96.09
ATOM	4996	CA	ALA	A	816	32.261	30.519	8.151	1.00	96.29
ATOM	4997	CB	ALA	A	816	31.379	30.008	7.018	1.00	94.97
ATOM	4998	C	ALA	A	816	33.087	29.379	8.732	1.00	96.72
ATOM	4999	O	ALA	A	816	33.967	28.829	8.070	1.00	97.42
ATOM	5000	N	ALA	A	817	32.779	29.039	9.981	1.00	98.13
ATOM	5001	CA	ALA	A	817	33.462	27.983	10.726	1.00	98.93
ATOM	5002	CB	ALA	A	817	32.946	27.957	12.160	1.00	99.14
ATOM	5003	C	ALA	A	817	33.289	26.611	10.093	1.00	99.65
ATOM	5004	O	ALA	A	817	33.178	26.489	8.875	1.00	98.83
ATOM	5005	N	ALA	A	818	33.262	25.580	10.937	1.00	101.12
ATOM	5006	CA	ALA	A	818	33.099	24.201	10.479	1.00	102.64
ATOM	5007	CB	ALA	A	818	31.628	23.923	10.139	1.00	102.05
ATOM	5008	C	ALA	A	818	33.979	23.946	9.261	1.00	103.58
ATOM	5009	O	ALA	A	818	35.175	23.679	9.404	1.00	103.89
ATOM	5010	N	ALA	A	819	33.382	24.039	8.072	1.00	103.66
ATOM	5011	CA	ALA	A	819	34.094	23.824	6.817	1.00	103.17
ATOM	5012	CB	ALA	A	819	34.633	25.144	6.287	1.00	101.98
ATOM	5013	C	ALA	A	819	35.230	22.830	7.006	1.00	103.60
ATOM	5014	O	ALA	A	819	36.348	23.044	6.539	1.00	101.87
ATOM	5015	N	ALA	A	820	34.930	21.751	7.723	1.00	105.51
ATOM	5016	CA	ALA	A	820	35.899	20.694	7.979	1.00	106.98
ATOM	5017	CB	ALA	A	820	35.620	20.031	9.327	1.00	105.25
ATOM	5018	C	ALA	A	820	35.726	19.692	6.847	1.00	107.93
ATOM	5019	O	ALA	A	820	36.635	18.925	6.529	1.00	108.45
ATOM	5020	N	ALA	A	821	34.544	19.720	6.240	1.00	109.32
ATOM	5021	CA	ALA	A	821	34.219	18.836	5.128	1.00	111.30
ATOM	5022	CB	ALA	A	821	32.719	18.891	4.835	1.00	112.18
ATOM	5023	C	ALA	A	821	35.015	19.263	3.898	1.00	111.97
ATOM	5024	O	ALA	A	821	35.435	18.427	3.093	1.00	113.00
ATOM	5025	N	ALA	A	822	35.210	20.571	3.754	1.00	111.37
ATOM	5026	CA	ALA	A	822	35.976	21.100	2.633	1.00	110.42
ATOM	5027	CB	ALA	A	822	35.818	22.614	2.552	1.00	109.77
ATOM	5028	C	ALA	A	822	37.434	20.727	2.873	1.00	109.52
ATOM	5029	O	ALA	A	822	38.244	20.695	1.946	1.00	109.15
ATOM	5030	N	ALA	A	823	37.751	20.438	4.132	1.00	108.52
ATOM	5031	CA	ALA	A	823	39.097	20.051	4.527	1.00	108.63
ATOM	5032	CB	ALA	A	823	39.278	20.242	6.025	1.00	107.76
ATOM	5033	C	ALA	A	823	39.338	18.596	4.155	1.00	109.71
ATOM	5034	O	ALA	A	823	38.480	18.018	3.456	1.00	110.54
ATOM	5035	OXT	ALA	A	823	40.383	18.049	4.563	1.00	110.87
TER	5036		ALA	A	823					

191/396

Figure 2A-91

ATOM	5037	CB	ALA	A	661	59.666	27.186	11.041	1.00	84.01
ATOM	5038	C	ALA	A	661	58.469	25.654	9.448	1.00	85.84
ATOM	5039	O	ALA	A	661	57.373	26.047	9.048	1.00	86.25
ATOM	5040	N	ALA	A	661	59.695	24.735	11.439	1.00	85.16
ATOM	5041	CA	ALA	A	661	58.884	25.875	10.907	1.00	86.13
ATOM	5042	N	ALA	A	662	59.335	25.027	8.654	1.00	85.55
ATOM	5043	CA	ALA	A	662	59.013	24.770	7.254	1.00	85.41
ATOM	5044	CB	ALA	A	662	60.252	24.279	6.501	1.00	84.99
ATOM	5045	C	ALA	A	662	57.887	23.743	7.155	1.00	85.74
ATOM	5046	O	ALA	A	662	57.282	23.562	6.096	1.00	86.37
ATOM	5047	N	ALA	A	663	57.613	23.065	8.265	1.00	85.70
ATOM	5048	CA	ALA	A	663	56.544	22.071	8.309	1.00	84.45
ATOM	5049	CB	ALA	A	663	56.746	21.134	9.497	1.00	84.91
ATOM	5050	C	ALA	A	663	55.217	22.823	8.438	1.00	83.95
ATOM	5051	O	ALA	A	663	54.207	22.446	7.834	1.00	83.85
ATOM	5052	N	ALA	A	664	55.237	23.897	9.225	1.00	82.45
ATOM	5053	CA	ALA	A	664	54.056	24.728	9.427	1.00	81.38
ATOM	5054	CB	ALA	A	664	54.364	25.852	10.412	1.00	82.68
ATOM	5055	C	ALA	A	664	53.607	25.313	8.093	1.00	80.12
ATOM	5056	O	ALA	A	664	52.430	25.223	7.739	1.00	79.10
ATOM	5057	N	ALA	A	665	54.550	25.909	7.360	1.00	78.65
ATOM	5058	CA	ALA	A	665	54.256	26.511	6.058	1.00	78.12
ATOM	5059	CB	ALA	A	665	55.549	26.977	5.368	1.00	76.58
ATOM	5060	C	ALA	A	665	53.555	25.492	5.189	1.00	77.85
ATOM	5061	O	ALA	A	665	52.584	25.812	4.496	1.00	77.63
ATOM	5062	N	ALA	A	666	54.066	24.263	5.236	1.00	77.86
ATOM	5063	CA	ALA	A	666	53.517	23.153	4.471	1.00	76.13
ATOM	5064	CB	ALA	A	666	54.337	21.890	4.730	1.00	76.84
ATOM	5065	C	ALA	A	666	52.070	22.935	4.880	1.00	74.69
ATOM	5066	O	ALA	A	666	51.154	22.974	4.046	1.00	73.80
ATOM	5067	N	ALA	A	667	51.862	22.714	6.172	1.00	73.11
ATOM	5068	CA	ALA	A	667	50.513	22.498	6.675	1.00	74.08
ATOM	5069	CB	ALA	A	667	50.523	22.382	8.200	1.00	73.93
ATOM	5070	C	ALA	A	667	49.611	23.644	6.243	1.00	73.74
ATOM	5071	O	ALA	A	667	48.593	23.422	5.586	1.00	74.48
ATOM	5072	N	ALA	A	668	49.997	24.869	6.599	1.00	71.85
ATOM	5073	CA	ALA	A	668	49.210	26.050	6.262	1.00	69.88
ATOM	5074	CB	ALA	A	668	49.905	27.314	6.768	1.00	71.15
ATOM	5075	C	ALA	A	668	48.974	26.146	4.769	1.00	68.70
ATOM	5076	O	ALA	A	668	47.885	26.516	4.329	1.00	68.07
ATOM	5077	N	ALA	A	669	49.996	25.806	3.991	1.00	68.76
ATOM	5078	CA	ALA	A	669	49.889	25.862	2.538	1.00	70.37
ATOM	5079	CB	ALA	A	669	51.259	25.669	1.902	1.00	67.36
ATOM	5080	C	ALA	A	669	48.908	24.810	2.023	1.00	71.23
ATOM	5081	O	ALA	A	669	48.178	25.048	1.062	1.00	70.12
ATOM	5082	N	ALA	A	670	48.891	23.648	2.669	1.00	74.14
ATOM	5083	CA	ALA	A	670	47.987	22.569	2.269	1.00	77.29
ATOM	5084	CB	ALA	A	670	48.454	21.249	2.866	1.00	78.77
ATOM	5085	C	ALA	A	670	46.553	22.871	2.714	1.00	78.97
ATOM	5086	O	ALA	A	670	45.618	22.806	1.907	1.00	80.07
ATOM	5087	N	ALA	A	671	46.382	23.198	3.996	1.00	78.67
ATOM	5088	CA	ALA	A	671	45.061	23.523	4.528	1.00	79.38
ATOM	5089	CB	ALA	A	671	45.173	24.059	5.952	1.00	79.67
ATOM	5090	C	ALA	A	671	44.456	24.574	3.618	1.00	79.75
ATOM	5091	O	ALA	A	671	43.265	24.539	3.316	1.00	80.37
ATOM	5092	N	ALA	A	672	45.295	25.506	3.175	1.00	80.05

Figure 2A-92

ATOM	5093	CA	ALA	A	672	44.861	26.567	2.279	1.00	79.86
ATOM	5094	CB	ALA	A	672	46.002	27.535	2.029	1.00	77.25
ATOM	5095	C	ALA	A	672	44.399	25.948	0.967	1.00	81.15
ATOM	5096	O	ALA	A	672	43.412	26.385	0.376	1.00	79.85
ATOM	5097	N	ALA	A	673	45.128	24.930	0.511	1.00	83.96
ATOM	5098	CA	ALA	A	673	44.778	24.243	-0.727	1.00	85.06
ATOM	5099	CB	ALA	A	673	45.696	23.043	-0.946	1.00	85.19
ATOM	5100	C	ALA	A	673	43.332	23.785	-0.593	1.00	86.03
ATOM	5101	O	ALA	A	673	42.505	24.007	-1.483	1.00	85.48
ATOM	5102	N	ALA	A	674	43.030	23.163	0.542	1.00	86.73
ATOM	5103	CA	ALA	A	674	41.680	22.685	0.805	1.00	88.01
ATOM	5104	CB	ALA	A	674	41.607	22.066	2.190	1.00	86.87
ATOM	5105	C	ALA	A	674	40.681	23.833	0.689	1.00	89.20
ATOM	5106	O	ALA	A	674	39.610	23.676	0.103	1.00	91.11
ATOM	5107	N	ALA	A	675	41.034	24.990	1.237	1.00	89.43
ATOM	5108	CA	ALA	A	675	40.145	26.142	1.181	1.00	89.60
ATOM	5109	CB	ALA	A	675	40.811	27.359	1.813	1.00	89.15
ATOM	5110	C	ALA	A	675	39.767	26.438	-0.262	1.00	89.30
ATOM	5111	O	ALA	A	675	38.592	26.398	-0.620	1.00	88.39
ATOM	5112	N	ALA	A	676	40.769	26.730	-1.087	1.00	90.54
ATOM	5113	CA	ALA	A	676	40.532	27.029	-2.496	1.00	91.48
ATOM	5114	CB	ALA	A	676	41.858	27.289	-3.212	1.00	90.37
ATOM	5115	C	ALA	A	676	39.802	25.849	-3.135	1.00	92.43
ATOM	5116	O	ALA	A	676	39.113	26.006	-4.148	1.00	91.27
ATOM	5117	N	ALA	A	677	39.955	24.674	-2.525	1.00	93.14
ATOM	5118	CA	ALA	A	677	39.310	23.452	-3.005	1.00	95.14
ATOM	5119	CB	ALA	A	677	40.109	22.225	-2.555	1.00	94.86
ATOM	5120	C	ALA	A	677	37.865	23.358	-2.498	1.00	95.64
ATOM	5121	O	ALA	A	677	37.394	22.279	-2.121	1.00	94.80
ATOM	5122	N	ALA	A	678	37.179	24.501	-2.485	1.00	95.00
ATOM	5123	CA	ALA	A	678	35.790	24.585	-2.048	1.00	93.78
ATOM	5124	CB	ALA	A	678	35.680	25.390	-0.760	1.00	92.80
ATOM	5125	C	ALA	A	678	35.000	25.259	-3.157	1.00	93.51
ATOM	5126	O	ALA	A	678	33.960	25.857	-2.919	1.00	94.27
ATOM	5127	N	ALA	A	679	35.522	25.165	-4.373	1.00	93.82
ATOM	5128	CA	ALA	A	679	34.885	25.735	-5.556	1.00	94.38
ATOM	5129	CB	ALA	A	679	33.631	24.916	-5.921	1.00	94.31
ATOM	5130	C	ALA	A	679	34.521	27.213	-5.417	1.00	93.19
ATOM	5131	O	ALA	A	679	33.579	27.563	-4.705	1.00	91.97
ATOM	5132	N	ALA	A	680	35.277	28.062	-6.113	1.00	92.48
ATOM	5133	CA	ALA	A	680	35.067	29.512	-6.126	1.00	92.55
ATOM	5134	CB	ALA	A	680	34.510	29.990	-4.785	1.00	92.83
ATOM	5135	C	ALA	A	680	36.365	30.257	-6.445	1.00	92.62
ATOM	5136	O	ALA	A	680	37.452	29.674	-6.425	1.00	92.57
ATOM	5137	N	ALA	A	686	36.243	31.550	-6.739	1.00	92.39
ATOM	5138	CA	ALA	A	686	37.400	32.387	-7.056	1.00	91.65
ATOM	5139	CB	ALA	A	686	36.935	33.702	-7.698	1.00	91.64
ATOM	5140	C	ALA	A	686	38.243	32.683	-5.812	1.00	90.07
ATOM	5141	O	ALA	A	686	39.345	33.225	-5.918	1.00	90.62
ATOM	5142	N	ALA	A	687	37.723	32.321	-4.641	1.00	87.82
ATOM	5143	CA	ALA	A	687	38.414	32.549	-3.369	1.00	85.42
ATOM	5144	CB	ALA	A	687	37.574	31.993	-2.208	1.00	84.04
ATOM	5145	C	ALA	A	687	39.825	31.947	-3.337	1.00	82.52
ATOM	5146	O	ALA	A	687	39.996	30.735	-3.188	1.00	80.85
ATOM	5147	N	ALA	A	688	40.828	32.814	-3.457	1.00	78.86
ATOM	5148	CA	ALA	A	688	42.226	32.397	-3.460	1.00	75.57

193/396

Figure 2A-93

ATOM	5149	CB	ALA	A	688	43.016	33.293	-4.412	1.00	73.70
ATOM	5150	C	ALA	A	688	42.881	32.396	-2.068	1.00	73.62
ATOM	5151	O	ALA	A	688	43.739	33.225	-1.778	1.00	71.05
ATOM	5152	N	ALA	A	689	42.482	31.456	-1.216	1.00	72.22
ATOM	5153	CA	ALA	A	689	43.043	31.354	0.127	1.00	72.53
ATOM	5154	CB	ALA	A	689	42.452	30.145	0.848	1.00	72.48
ATOM	5155	C	ALA	A	689	44.566	31.232	0.047	1.00	73.62
ATOM	5156	O	ALA	A	689	45.122	31.035	-1.037	1.00	75.15
ATOM	5157	N	ALA	A	690	45.240	31.346	1.189	1.00	70.89
ATOM	5158	CA	ALA	A	690	46.694	31.253	1.209	1.00	69.13
ATOM	5159	CB	ALA	A	690	47.286	32.538	0.693	1.00	72.34
ATOM	5160	C	ALA	A	690	47.248	30.939	2.595	1.00	68.65
ATOM	5161	O	ALA	A	690	46.533	31.007	3.589	1.00	70.52
ATOM	5162	N	ALA	A	691	48.524	30.585	2.652	1.00	67.57
ATOM	5163	CA	ALA	A	691	49.172	30.250	3.916	1.00	68.97
ATOM	5164	CB	ALA	A	691	50.676	30.029	3.689	1.00	70.11
ATOM	5165	C	ALA	A	691	48.956	31.347	4.960	1.00	67.51
ATOM	5166	O	ALA	A	691	48.705	31.071	6.138	1.00	65.52
ATOM	5167	N	ALA	A	692	49.057	32.592	4.511	1.00	67.55
ATOM	5168	CA	ALA	A	692	48.886	33.746	5.383	1.00	68.38
ATOM	5169	CB	ALA	A	692	49.425	35.010	4.695	1.00	69.15
ATOM	5170	C	ALA	A	692	47.426	33.936	5.771	1.00	66.99
ATOM	5171	O	ALA	A	692	47.119	34.658	6.717	1.00	66.88
ATOM	5172	N	ALA	A	693	46.525	33.286	5.044	1.00	67.07
ATOM	5173	CA	ALA	A	693	45.100	33.395	5.343	1.00	65.70
ATOM	5174	CB	ALA	A	693	44.288	33.390	4.055	1.00	63.93
ATOM	5175	C	ALA	A	693	44.648	32.263	6.271	1.00	65.70
ATOM	5176	O	ALA	A	693	43.459	32.102	6.530	1.00	65.39
ATOM	5177	N	ALA	A	694	45.608	31.485	6.767	1.00	67.00
ATOM	5178	CA	ALA	A	694	45.336	30.379	7.690	1.00	67.90
ATOM	5179	CB	ALA	A	694	45.831	29.040	7.094	1.00	66.14
ATOM	5180	C	ALA	A	694	46.085	30.700	8.979	1.00	67.31
ATOM	5181	O	ALA	A	694	47.305	30.581	9.038	1.00	68.10
ATOM	5182	N	ALA	A	695	45.348	31.098	10.012	1.00	69.03
ATOM	5183	CA	ALA	A	695	45.940	31.500	11.289	1.00	68.70
ATOM	5184	CB	ALA	A	695	45.176	32.718	11.829	1.00	67.51
ATOM	5185	C	ALA	A	695	46.043	30.433	12.377	1.00	69.22
ATOM	5186	O	ALA	A	695	45.034	29.949	12.880	1.00	69.79
ATOM	5187	N	ALA	A	696	47.275	30.099	12.755	1.00	71.16
ATOM	5188	CA	ALA	A	696	47.545	29.101	13.790	1.00	72.12
ATOM	5189	CB	ALA	A	696	48.773	28.269	13.405	1.00	69.43
ATOM	5190	C	ALA	A	696	47.759	29.756	15.155	1.00	73.86
ATOM	5191	O	ALA	A	696	48.389	30.807	15.252	1.00	75.03
ATOM	5192	N	ALA	A	697	47.230	29.126	16.202	1.00	76.93
ATOM	5193	CA	ALA	A	697	47.345	29.646	17.563	1.00	79.23
ATOM	5194	CB	ALA	A	697	46.005	30.212	18.020	1.00	77.88
ATOM	5195	C	ALA	A	697	47.813	28.563	18.536	1.00	81.98
ATOM	5196	O	ALA	A	697	47.988	27.401	18.149	1.00	82.69
ATOM	5197	N	ALA	A	698	47.999	28.944	19.800	1.00	84.10
ATOM	5198	CA	ALA	A	698	48.463	28.017	20.840	1.00	86.52
ATOM	5199	CB	ALA	A	698	47.559	26.793	20.911	1.00	84.65
ATOM	5200	C	ALA	A	698	49.911	27.612	20.530	1.00	88.44
ATOM	5201	O	ALA	A	698	50.753	28.479	20.285	1.00	91.04
ATOM	5202	N	ALA	A	699	50.209	26.317	20.533	1.00	87.97
ATOM	5203	CA	ALA	A	699	51.561	25.842	20.228	1.00	87.93
ATOM	5204	CB	ALA	A	699	51.977	26.317	18.830	1.00	86.32

194/396

Figure 2A-94

ATOM	5205	C	ALA	A	699	52.646	26.230	21.249	1.00	88.10
ATOM	5206	O	ALA	A	699	52.376	27.027	22.177	1.00	89.43
ATOM	5207	OXT	ALA	A	699	53.782	25.738	21.099	1.00	87.19
TER	5208		ALA	A	699					
ATOM	5209	CB	ALA	A	701	54.820	10.723	15.170	1.00	113.30
ATOM	5210	C	ALA	A	701	53.011	12.130	16.177	1.00	114.47
ATOM	5211	O	ALA	A	701	53.725	13.099	15.911	1.00	114.81
ATOM	5212	N	ALA	A	701	52.456	10.240	14.647	1.00	113.76
ATOM	5213	CA	ALA	A	701	53.392	10.728	15.702	1.00	114.11
ATOM	5214	N	ALA	A	702	51.886	12.216	16.888	1.00	115.06
ATOM	5215	CA	ALA	A	702	51.348	13.466	17.438	1.00	115.24
ATOM	5216	CB	ALA	A	702	52.479	14.395	17.903	1.00	114.90
ATOM	5217	C	ALA	A	702	50.449	14.191	16.433	1.00	115.33
ATOM	5218	O	ALA	A	702	50.313	13.763	15.285	1.00	115.51
ATOM	5219	N	ALA	A	703	49.831	15.282	16.883	1.00	114.69
ATOM	5220	CA	ALA	A	703	48.918	16.102	16.074	1.00	114.02
ATOM	5221	CB	ALA	A	703	49.526	16.372	14.698	1.00	113.88
ATOM	5222	C	ALA	A	703	47.516	15.494	15.935	1.00	113.47
ATOM	5223	O	ALA	A	703	46.764	15.436	16.900	1.00	113.45
ATOM	5224	N	ALA	A	704	47.166	15.057	14.730	1.00	113.33
ATOM	5225	CA	ALA	A	704	45.861	14.438	14.465	1.00	113.07
ATOM	5226	CB	ALA	A	704	45.508	13.461	15.588	1.00	112.95
ATOM	5227	C	ALA	A	704	44.714	15.463	14.268	1.00	112.74
ATOM	5228	O	ALA	A	704	44.599	16.452	14.997	1.00	112.35
ATOM	5229	N	ALA	A	705	43.861	15.186	13.279	1.00	113.04
ATOM	5230	CA	ALA	A	705	42.722	16.025	12.867	1.00	112.53
ATOM	5231	CB	ALA	A	705	41.902	15.283	11.800	1.00	112.83
ATOM	5232	C	ALA	A	705	41.779	16.555	13.945	1.00	112.42
ATOM	5233	O	ALA	A	705	42.113	16.439	15.138	1.00	112.81
ATOM	5234	OXT	ALA	A	705	40.706	17.105	13.584	1.00	112.33
TER	5235		ALA	A	705					
ATOM	5236	OH2	TIP	S	1	49.545	45.322	21.437	1.00	22.81
ATOM	5237	OH2	TIP	S	2	46.430	59.242	7.263	1.00	29.64
ATOM	5238	OH2	TIP	S	3	45.576	47.117	26.121	1.00	37.00
ATOM	5239	OH2	TIP	S	4	53.476	43.446	15.548	1.00	42.04
ATOM	5240	OH2	TIP	S	5	39.174	66.723	40.345	1.00	45.69
ATOM	5241	OH2	TIP	S	6	57.397	64.704	34.702	1.00	43.87
ATOM	5242	OH2	TIP	S	7	49.118	35.268	20.766	1.00	51.35
ATOM	5243	OH2	TIP	S	8	38.449	72.836	48.687	1.00	55.26
ATOM	5244	OH2	TIP	S	9	65.177	44.872	33.810	1.00	43.34
ATOM	5245	OH2	TIP	S	10	61.734	51.551	33.715	1.00	42.60
ATOM	5246	OH2	TIP	S	11	44.164	48.376	28.154	1.00	35.76
ATOM	5247	OH2	TIP	S	12	52.074	57.442	18.699	1.00	47.25
ATOM	5248	OH2	TIP	S	13	46.785	57.036	23.083	1.00	45.33
ATOM	5249	OH2	TIP	S	14	67.706	76.390	33.214	1.00	49.16
ATOM	5250	OH2	TIP	S	15	62.454	54.498	34.604	1.00	62.08
ATOM	5251	OH2	TIP	S	16	65.272	76.797	36.314	1.00	46.51
ATOM	5252	OH2	TIP	S	17	39.439	36.009	27.893	1.00	49.35
ATOM	5253	OH2	TIP	S	18	50.040	55.390	30.125	1.00	43.51
ATOM	5254	OH2	TIP	S	19	64.046	56.191	33.054	1.00	45.90
ATOM	5255	OH2	TIP	S	20	54.043	69.195	29.050	1.00	53.33
ATOM	5256	OH2	TIP	S	21	40.753	55.764	24.327	1.00	43.74
ATOM	5257	OH2	TIP	S	22	58.549	57.533	15.451	1.00	47.74
ATOM	5258	OH2	TIP	S	23	60.253	65.381	36.455	1.00	41.32
ATOM	5259	OH2	TIP	S	24	61.698	50.224	24.078	1.00	37.01
ATOM	5260	OH2	TIP	S	25	61.613	47.466	6.953	1.00	46.28

195/396

Figure 2A-95

ATOM	5261	OH2	TIP	S	26	39.064	68.331	38.385	1.00	40.55
ATOM	5262	OH2	TIP	S	27	48.412	57.903	45.042	1.00	44.00
ATOM	5263	OH2	TIP	S	28	60.806	42.181	36.580	1.00	47.39
ATOM	5264	OH2	TIP	S	29	51.139	59.951	50.711	1.00	50.91
ATOM	5265	OH2	TIP	S	30	45.463	55.515	18.760	1.00	45.46
ATOM	5266	OH2	TIP	S	31	62.718	73.493	50.939	1.00	59.08
ATOM	5267	OH2	TIP	S	32	45.978	46.445	21.875	1.00	43.74
ATOM	5268	OH2	TIP	S	33	72.481	42.488	29.968	1.00	49.77
ATOM	5269	OH2	TIP	S	34	36.393	42.674	35.604	1.00	49.03
ATOM	5270	OH2	TIP	S	35	52.413	74.700	55.230	1.00	68.84
ATOM	5271	OH2	TIP	S	36	67.542	43.906	36.141	1.00	57.99
ATOM	5272	OH2	TIP	S	37	49.414	57.114	23.258	1.00	49.15
ATOM	5273	OH2	TIP	S	38	37.080	62.007	45.468	1.00	47.38
ATOM	5274	OH2	TIP	S	39	29.740	41.211	41.369	1.00	66.20
ATOM	5275	OH2	TIP	S	40	51.029	43.063	41.914	1.00	61.41
ATOM	5276	OH2	TIP	S	41	43.298	56.630	18.617	1.00	47.33
ATOM	5277	OH2	TIP	S	42	49.385	62.046	50.513	1.00	55.22
ATOM	5278	OH2	TIP	S	43	63.737	57.222	28.504	1.00	44.91
ATOM	5279	OH2	TIP	S	44	66.689	61.391	43.589	1.00	43.43
ATOM	5280	OH2	TIP	S	45	45.233	43.402	37.391	1.00	60.70
ATOM	5281	OH2	TIP	S	46	57.633	79.130	41.470	1.00	49.30
ATOM	5282	OH2	TIP	S	47	41.624	49.507	20.692	1.00	40.92
ATOM	5283	OH2	TIP	S	48	31.085	62.069	24.688	1.00	62.98
ATOM	5284	OH2	TIP	S	49	56.072	49.126	49.409	1.00	62.80
ATOM	5285	OH2	TIP	S	50	52.128	89.974	43.293	1.00	65.58
ATOM	5286	OH2	TIP	S	51	58.050	55.804	42.785	1.00	42.08
ATOM	5287	OH2	TIP	S	52	27.159	50.867	25.633	1.00	54.85
ATOM	5288	OH2	TIP	S	53	65.256	66.995	45.459	1.00	41.70
ATOM	5289	OH2	TIP	S	54	77.914	73.472	41.334	1.00	58.79
ATOM	5290	OH2	TIP	S	55	32.437	67.370	39.272	1.00	60.99
ATOM	5291	OH2	TIP	S	56	63.024	46.701	48.192	1.00	64.29
ATOM	5292	OH2	TIP	S	57	58.950	40.116	11.627	1.00	46.79
ATOM	5293	OH2	TIP	S	58	50.939	64.827	32.040	1.00	58.45
ATOM	5294	OH2	TIP	S	59	70.989	83.801	40.551	1.00	69.27
ATOM	5295	OH2	TIP	S	60	57.886	33.984	32.530	1.00	60.12
ATOM	5296	OH2	TIP	S	61	79.175	83.227	24.694	1.00	63.71
ATOM	5297	OH2	TIP	S	62	72.082	57.977	14.047	1.00	69.19
ATOM	5298	OH2	TIP	S	63	73.538	42.017	25.376	1.00	53.18
ATOM	5299	OH2	TIP	S	64	47.388	39.741	9.561	1.00	50.71
ATOM	5300	OH2	TIP	S	65	35.330	48.191	0.775	1.00	66.09
ATOM	5301	OH2	TIP	S	66	69.794	46.455	40.493	1.00	52.24
ATOM	5302	OH2	TIP	S	67	57.631	83.285	34.350	1.00	49.94
ATOM	5303	OH2	TIP	S	68	52.038	62.712	30.807	1.00	57.14
ATOM	5304	OH2	TIP	S	69	43.073	85.517	22.282	1.00	56.08
ATOM	5305	OH2	TIP	S	70	62.355	45.818	9.059	1.00	50.97
ATOM	5306	OH2	TIP	S	71	40.439	57.423	9.123	1.00	50.76
ATOM	5307	OH2	TIP	S	72	65.467	56.496	26.919	1.00	66.20
ATOM	5308	OH2	TIP	S	73	86.710	72.670	26.417	1.00	65.41
ATOM	5309	OH2	TIP	S	74	62.405	88.458	33.079	1.00	47.85
ATOM	5310	OH2	TIP	S	75	68.838	73.543	48.200	1.00	70.48
ATOM	5311	OH2	TIP	S	76	29.142	41.201	23.270	1.00	61.23
ATOM	5312	OH2	TIP	S	77	52.651	30.829	11.843	1.00	70.30
ATOM	5313	OH2	TIP	S	78	38.003	52.214	6.763	1.00	63.32
ATOM	5314	OH2	TIP	S	79	76.403	64.571	23.916	1.00	63.89
ATOM	5315	OH2	TIP	S	80	43.479	61.575	15.985	1.00	85.72
ATOM	5316	OH2	TIP	S	81	53.654	48.191	4.663	1.00	63.00

196/396

Figure 2A-96

ATOM	5317	OH2	TIP	S	82	31.209	38.380	40.229	1.00	70.02
ATOM	5318	OH2	TIP	S	83	51.898	83.417	38.956	1.00	51.39
ATOM	5319	OH2	TIP	S	84	70.128	41.343	33.653	1.00	58.52
ATOM	5320	OH2	TIP	S	85	74.485	76.907	37.609	1.00	56.95
ATOM	5321	OH2	TIP	S	86	36.947	60.992	48.081	1.00	56.20
ATOM	5322	OH2	TIP	S	87	52.463	60.298	26.599	1.00	44.84
ATOM	5323	OH2	TIP	S	88	52.707	55.761	10.530	1.00	36.69
ATOM	5324	OH2	TIP	S	89	67.583	74.344	32.226	1.00	68.81
ATOM	5325	OH2	TIP	S	90	46.250	36.715	10.391	1.00	59.57
ATOM	5326	OH2	TIP	S	91	58.356	70.223	30.881	1.00	57.72
ATOM	5327	OH2	TIP	S	92	51.914	58.286	11.640	1.00	46.27
ATOM	5328	OH2	TIP	S	93	59.867	55.969	32.841	1.00	49.22
ATOM	5329	OH2	TIP	S	94	49.249	47.645	23.845	1.00	48.71
ATOM	5330	OH2	TIP	S	95	61.800	84.879	17.641	1.00	71.73
ATOM	5331	OH2	TIP	S	96	43.575	60.453	26.576	1.00	53.52
ATOM	5332	OH2	TIP	S	97	58.486	61.209	25.335	1.00	57.10
ATOM	5333	OH2	TIP	S	98	52.168	67.076	28.758	1.00	60.64
ATOM	5334	OH2	TIP	S	99	56.001	71.181	28.774	1.00	52.88
ATOM	5335	OH2	TIP	S	100	49.299	32.768	21.132	1.00	67.03
ATOM	5336	OH2	TIP	S	101	20.746	59.774	45.039	1.00	68.19
ATOM	5337	OH2	TIP	S	102	63.385	49.673	6.618	1.00	58.08
ATOM	5338	OH2	TIP	S	103	46.346	57.955	20.559	1.00	51.67
ATOM	5339	OH2	TIP	S	104	56.283	61.956	24.884	1.00	72.77
ATOM	5340	OH2	TIP	S	105	45.799	61.126	27.776	1.00	55.88
ATOM	5341	OH2	TIP	S	106	89.871	54.413	31.214	1.00	76.61
ATOM	5342	OH2	TIP	S	107	39.526	53.664	5.463	1.00	67.13
ATOM	5343	OH2	TIP	S	108	60.919	85.551	19.801	1.00	79.10
ATOM	5344	OH2	TIP	S	109	53.095	81.481	40.707	1.00	96.38
ATOM	5345	OH2	TIP	S	110	47.434	34.668	25.158	1.00	63.49
ATOM	5346	OH2	TIP	S	111	61.405	85.277	29.329	1.00	54.00
ATOM	5347	OH2	TIP	S	112	34.412	40.520	34.891	1.00	61.78
ATOM	5348	OH2	TIP	S	113	45.435	30.596	-3.577	1.00	66.14
ATOM	5349	OH2	TIP	S	114	62.179	69.082	43.392	1.00	46.34
ATOM	5350	OH2	TIP	S	115	61.044	48.007	48.516	1.00	63.93
ATOM	5351	OH2	TIP	S	116	28.016	74.646	28.335	1.00	65.79
ATOM	5352	OH2	TIP	S	117	67.037	59.393	42.026	1.00	45.97
ATOM	5353	OH2	TIP	S	118	101.749	64.917	50.857	1.00	57.51
ATOM	5354	OH2	TIP	S	119	47.038	35.531	12.699	1.00	53.34
ATOM	5355	OH2	TIP	S	120	46.432	59.634	23.553	1.00	59.36
ATOM	5356	OH2	TIP	S	121	70.309	58.874	15.612	1.00	75.99
ATOM	5357	OH2	TIP	S	122	63.948	54.921	18.151	1.00	45.13
ATOM	5358	OH2	TIP	S	123	23.442	50.302	29.826	1.00	64.78
ATOM	5359	OH2	TIP	S	124	70.237	49.693	43.253	1.00	62.35
ATOM	5360	OH2	TIP	S	125	63.252	79.627	44.372	1.00	64.42
ATOM	5361	OH2	TIP	S	126	69.591	61.709	44.302	1.00	48.16
ATOM	5362	OH2	TIP	S	127	74.744	75.727	21.968	1.00	57.06
ATOM	5363	OH2	TIP	S	128	67.375	79.057	15.093	1.00	70.18
ATOM	5364	OH2	TIP	S	129	28.201	37.666	43.253	1.00	77.95
ATOM	5365	OH2	TIP	S	130	46.238	63.550	31.339	1.00	61.10
ATOM	5366	OH2	TIP	S	131	70.323	40.312	30.964	1.00	56.75
ATOM	5367	OH2	TIP	S	132	27.856	77.993	33.358	1.00	68.63
ATOM	5368	OH2	TIP	S	133	82.160	46.121	17.111	1.00	65.25
ATOM	5369	OH2	TIP	S	134	85.327	58.267	38.423	1.00	74.59
ATOM	5370	OH2	TIP	S	135	62.797	35.947	15.959	1.00	57.78
ATOM	5371	OH2	TIP	S	136	70.557	51.932	47.024	1.00	50.26
ATOM	5372	OH2	TIP	S	137	41.834	79.830	37.050	1.00	49.42

197/396

Figure 2A-97

ATOM	5373	OH2	TIP	S	138	25.075	57.946	43.494	1.00	62.02
ATOM	5374	OH2	TIP	S	139	49.849	60.012	52.953	1.00	65.47
ATOM	5375	OH2	TIP	S	140	46.228	56.970	0.442	1.00	61.04
ATOM	5376	OH2	TIP	S	141	39.867	55.021	49.742	1.00	67.46
ATOM	5377	OH2	TIP	S	142	26.137	54.521	28.645	1.00	57.03
ATOM	5378	OH2	TIP	S	143	54.744	56.972	4.347	1.00	63.52
ATOM	5379	OH2	TIP	S	144	72.551	60.558	46.556	1.00	70.13
ATOM	5380	OH2	TIP	S	145	53.103	57.696	13.998	1.00	46.17
ATOM	5381	OH2	TIP	S	146	49.609	68.736	53.951	1.00	70.72
ATOM	5382	OH2	TIP	S	147	51.842	88.154	26.297	1.00	80.55
ATOM	5383	OH2	TIP	S	148	52.295	34.105	31.446	1.00	64.43
ATOM	5384	OH2	TIP	S	149	65.771	48.152	7.469	1.00	67.41
ATOM	5385	OH2	TIP	S	150	64.845	75.303	26.789	1.00	67.02
ATOM	5386	OH2	TIP	S	151	31.517	53.943	13.065	1.00	60.23
ATOM	5387	OH2	TIP	S	152	24.466	50.588	27.185	1.00	59.50
ATOM	5388	OH2	TIP	S	153	26.997	77.809	43.088	1.00	72.83
ATOM	5389	OH2	TIP	S	154	41.880	53.224	-6.568	1.00	58.27
ATOM	5390	OH2	TIP	S	155	34.987	24.863	13.451	1.00	74.11
ATOM	5391	OH2	TIP	S	156	39.707	16.302	1.430	1.00	60.04
ATOM	5392	OH2	TIP	S	157	58.133	62.698	23.192	1.00	64.58
ATOM	5393	OH2	TIP	S	158	64.974	46.487	9.154	1.00	69.66
ATOM	5394	OH2	TIP	S	159	30.468	25.555	-4.755	1.00	63.94
ATOM	5395	OH2	TIP	S	160	70.439	59.658	43.446	1.00	53.70
ATOM	5396	OH2	TIP	S	161	71.225	40.547	25.618	1.00	61.80
ATOM	5397	OH2	TIP	S	162	49.787	34.114	24.375	1.00	62.93
ATOM	5398	OH2	TIP	S	163	50.558	60.878	28.233	1.00	75.90
ATOM	5399	OH2	TIP	S	164	51.300	58.040	21.406	1.00	68.53
ATOM	5400	OH2	TIP	S	165	52.553	60.603	10.791	1.00	60.70
ATOM	5401	OH2	TIP	S	166	64.908	45.104	47.522	1.00	66.71
ATOM	5402	OH2	TIP	S	167	59.572	68.152	31.727	1.00	88.82
ATOM	5403	OH2	TIP	S	168	61.089	65.260	33.564	1.00	66.27
ATOM	5404	OH2	TIP	S	169	65.053	57.085	19.063	1.00	52.24
ATOM	5405	OH2	TIP	S	170	78.141	85.223	23.463	1.00	71.25
ATOM	5406	OH2	TIP	S	171	30.921	42.779	33.082	1.00	54.68
ATOM	5407	OH2	TIP	S	172	78.008	77.003	47.812	1.00	60.40
ATOM	5408	OH2	TIP	S	173	52.953	69.613	20.177	1.00	68.71
ATOM	5409	OH2	TIP	S	174	44.851	40.637	37.415	1.00	93.18
ATOM	5410	OH2	TIP	S	175	32.363	68.427	37.128	1.00	68.91
ATOM	5411	OH2	TIP	S	176	21.535	58.149	42.965	1.00	75.76
ATOM	5412	OH2	TIP	S	177	73.147	58.653	44.906	1.00	55.90
ATOM	5413	OH2	TIP	S	178	44.298	48.610	30.952	1.00	45.47
ATOM	5414	OH2	TIP	S	179	68.210	72.267	33.291	1.00	82.79
ATOM	5415	OH2	TIP	S	180	64.575	57.877	30.906	1.00	55.74
ATOM	5416	OH2	TIP	S	181	68.974	63.943	42.760	1.00	63.53
ATOM	5417	OH2	TIP	S	182	29.990	68.185	39.130	1.00	88.91
ATOM	5418	OH2	TIP	S	183	65.633	50.484	5.013	1.00	85.14
ATOM	5419	OH2	TIP	S	184	63.305	82.091	39.855	1.00	57.51
ATOM	5420	OH2	TIP	S	185	45.405	58.277	51.657	1.00	67.82
ATOM	5421	OH2	TIP	S	186	50.432	73.475	25.286	1.00	81.07
ATOM	5422	OH2	TIP	S	187	62.153	85.489	11.340	1.00	72.58
ATOM	5423	OH2	TIP	S	188	54.629	55.369	2.331	1.00	72.10
ATOM	5424	OH2	TIP	S	189	60.230	86.440	12.553	1.00	64.27
ATOM	5425	OH2	TIP	S	190	24.113	77.326	34.487	1.00	77.84
ATOM	5426	OH2	TIP	S	191	64.861	58.321	22.765	1.00	56.79
ATOM	5427	OH2	TIP	S	192	36.546	69.221	38.424	1.00	61.47
ATOM	5428	OH2	TIP	S	193	65.223	35.438	15.702	1.00	67.34

198/396

Figure 2A-98

ATOM	5429	OH2	TIP	S	194	87.133	75.766	27.787	1.00	67.68
ATOM	5430	OH2	TIP	S	195	61.803	64.750	31.169	1.00	75.25
ATOM	5431	OH2	TIP	S	196	50.015	31.115	0.565	1.00	73.66
ATOM	5432	OH2	TIP	S	197	47.825	58.968	3.834	1.00	59.19
ATOM	5433	OH2	TIP	S	198	77.648	78.449	49.907	1.00	59.83
ATOM	5434	OH2	TIP	S	199	56.545	62.003	27.647	1.00	74.41
ATOM	5435	OH2	TIP	S	200	60.906	36.243	14.318	1.00	66.07
ATOM	5436	OH2	TIP	S	201	41.818	82.799	38.633	1.00	64.96
ATOM	5437	OH2	TIP	S	202	59.264	34.150	30.565	1.00	61.57
ATOM	5438	OH2	TIP	S	203	66.928	61.068	39.278	1.00	66.16
ATOM	5439	OH2	TIP	S	204	34.771	60.324	49.396	1.00	57.72
ATOM	5440	OH2	TIP	S	205	63.471	86.821	30.804	1.00	67.59
ATOM	5441	OH2	TIP	S	206	80.068	80.750	40.682	1.00	72.89
ATOM	5442	OH2	TIP	S	207	41.388	49.118	44.350	1.00	48.59
ATOM	5443	OH2	TIP	S	208	40.133	68.846	42.367	1.00	54.66
ATOM	5444	OH2	TIP	S	209	35.025	51.167	21.015	1.00	49.53
ATOM	5445	OH2	TIP	S	210	20.825	50.960	29.294	1.00	67.26
ATOM	5446	OH2	TIP	S	211	88.602	74.058	25.989	1.00	69.32
ATOM	5447	OH2	TIP	S	212	70.173	39.513	28.574	1.00	86.86
ATOM	5448	OH2	TIP	S	213	56.207	68.585	55.519	1.00	77.80
ATOM	5449	OH2	TIP	S	214	58.580	53.605	44.475	1.00	51.15
ATOM	5450	OH2	TIP	S	215	71.181	80.846	19.234	1.00	65.54
ATOM	5451	OH2	TIP	S	216	71.298	54.679	22.333	1.00	60.22
ATOM	5452	OH2	TIP	S	217	51.078	66.793	54.324	1.00	63.78
ATOM	5453	OH2	TIP	S	218	82.401	46.359	20.147	1.00	81.89
ATOM	5454	OH2	TIP	S	219	66.873	70.741	51.833	1.00	60.77
ATOM	5455	OH2	TIP	S	220	84.553	72.308	33.318	1.00	53.04
ATOM	5456	OH2	TIP	S	221	39.989	74.333	50.382	1.00	62.08
ATOM	5457	OH2	TIP	S	222	74.830	77.654	12.721	1.00	77.50
ATOM	5458	OH2	TIP	S	223	80.634	47.015	22.774	1.00	77.30
ATOM	5459	OH2	TIP	S	224	47.118	34.445	30.617	1.00	54.51
ATOM	5460	OH2	TIP	S	225	22.888	50.661	24.553	1.00	79.63
ATOM	5461	OH2	TIP	S	226	42.927	83.463	21.069	1.00	65.55
ATOM	5462	OH2	TIP	S	227	48.316	46.525	4.414	1.00	70.72
ATOM	5463	OH2	TIP	S	228	49.891	62.644	8.759	1.00	57.37
ATOM	5464	OH2	TIP	S	229	29.803	62.508	22.532	1.00	67.75
ATOM	5465	OH2	TIP	S	230	28.084	73.736	31.489	1.00	72.37
ATOM	5466	OH2	TIP	S	231	78.563	55.242	33.677	1.00	69.37
ATOM	5467	OH2	TIP	S	232	63.452	82.015	43.955	1.00	67.83
ATOM	5468	OH2	TIP	S	233	75.583	59.672	56.212	1.00	75.89
ATOM	5469	OH2	TIP	S	234	52.028	8.566	12.691	1.00	74.04
ATOM	5470	OH2	TIP	S	235	64.200	64.536	36.560	1.00	59.95
ATOM	5471	OH2	TIP	S	236	37.303	24.008	-5.092	1.00	73.19
ATOM	5472	OH2	TIP	S	237	18.881	57.883	45.897	1.00	72.90
ATOM	5473	OH2	TIP	S	238	58.391	63.966	30.390	1.00	85.96
ATOM	5474	OH2	TIP	S	239	31.256	23.376	-3.784	1.00	77.18
ATOM	5475	OH2	TIP	S	240	41.686	17.351	0.602	1.00	64.57
ATOM	5476	OH2	TIP	S	241	37.123	17.345	-0.521	1.00	59.57
ATOM	5477	OH2	TIP	S	242	35.536	53.935	20.852	1.00	65.03
ATOM	5478	OH2	TIP	S	243	37.504	16.270	1.902	1.00	74.58
ATOM	5479	OH2	TIP	S	244	69.385	60.818	38.067	1.00	74.22
ATOM	5480	OH2	TIP	S	245	47.307	62.027	23.014	1.00	88.79
ATOM	5481	OH2	TIP	S	246	42.050	15.408	2.627	1.00	62.77
ATOM	5482	OH2	TIP	S	247	48.067	12.150	13.784	1.00	82.24
ATOM	5483	OH2	TIP	S	248	48.364	62.410	19.477	1.00	89.54
ATOM	5484	OH2	TIP	S	249	49.644	33.763	1.920	1.00	65.25

199/396

Figure 2A-99

ATOM	5485	OH2	TIP	S	250	54.898	69.141	26.890	1.00	62.50
ATOM	5486	OH2	TIP	S	251	35.622	22.575	14.573	1.00	83.73
ATOM	5487	OH2	TIP	S	252	25.781	51.062	22.964	1.00	62.93
ATOM	5488	OH2	TIP	S	253	53.368	6.536	14.256	1.00	79.29
ATOM	5489	OH2	TIP	S	254	52.852	60.377	22.624	1.00	73.11
ATOM	5490	OH2	TIP	S	255	49.326	9.726	13.407	1.00	68.99
ATOM	5491	OH2	TIP	S	256	64.444	70.461	52.484	1.00	65.41
ATOM	5492	OH2	TIP	S	257	47.623	58.682	52.777	1.00	72.39
ATOM	5493	OH2	TIP	S	258	41.603	66.741	42.944	1.00	74.12
ATOM	5494	OH2	TIP	S	259	48.367	69.616	19.858	1.00	75.12
ATOM	5495	OH2	TIP	S	260	65.385	59.312	20.423	1.00	63.90
ATOM	5496	OH2	TIP	S	261	34.135	71.975	43.600	1.00	71.60
ATOM	5497	OH2	TIP	S	262	46.723	60.718	32.507	1.00	62.94
ATOM	5498	OH2	TIP	S	263	21.337	56.927	45.177	1.00	76.47
ATOM	5499	OH2	TIP	S	264	25.096	78.526	32.481	1.00	93.57
ATOM	5500	OH2	TIP	S	265	53.993	57.943	0.761	1.00	74.23
ATOM	5501	OH2	TIP	S	266	64.107	73.044	33.762	1.00	52.36
ATOM	5502	OH2	TIP	S	267	85.896	73.929	31.006	1.00	69.86
ATOM	5503	OH2	TIP	S	268	50.017	65.147	28.265	1.00	69.71
ATOM	5504	OH2	TIP	S	269	41.255	61.504	50.187	1.00	72.12
ATOM	5505	OH2	TIP	S	270	71.021	40.127	35.596	1.00	76.68
ATOM	5506	OH2	TIP	S	271	81.445	77.849	48.324	1.00	75.98
ATOM	5507	OH2	TIP	S	272	34.256	69.676	29.012	1.00	73.83
ATOM	5508	OH2	TIP	S	273	44.834	45.672	4.994	1.00	74.16
ATOM	5509	OH2	TIP	S	274	63.360	28.723	24.638	1.00	72.09
ATOM	5510	OH2	TIP	S	275	67.132	56.904	21.670	1.00	55.62
ATOM	5511	OH2	TIP	S	276	22.968	59.974	46.283	1.00	86.18
ATOM	5512	OH2	TIP	S	277	58.358	40.680	40.895	1.00	70.10
ATOM	5513	OH2	TIP	S	278	85.217	56.091	37.286	1.00	89.83
ATOM	5514	OH2	TIP	S	279	73.993	60.099	58.768	1.00	78.64
ATOM	5515	OH2	TIP	S	280	74.504	77.468	15.386	1.00	84.49
ATOM	5516	OH2	TIP	S	281	89.910	55.916	29.305	1.00	92.22
ATOM	5517	OH2	TIP	S	282	27.125	38.549	40.463	1.00	97.54
ATOM	5518	OH2	TIP	S	283	37.695	74.917	52.985	1.00	65.27
ATOM	5519	OH2	TIP	S	284	47.094	32.572	28.243	1.00	60.72
ATOM	5520	OH2	TIP	S	285	91.841	56.522	31.166	1.00	84.18
ATOM	5521	OH2	TIP	S	286	49.743	58.098	31.149	1.00	58.01
ATOM	5522	OH2	TIP	S	287	61.501	83.053	41.363	1.00	70.10
ATOM	5523	OH2	TIP	S	288	52.321	18.518	23.497	1.00	76.44
ATOM	5524	OH2	TIP	S	289	78.790	45.173	34.820	1.00	70.99
ATOM	5525	OH2	TIP	S	290	28.133	75.498	40.052	1.00	74.61
ATOM	5526	OH2	TIP	S	291	74.767	38.066	27.872	1.00	90.30
ATOM	5527	OH2	TIP	S	292	45.180	66.605	35.838	1.00	57.86
ATOM	5528	OH2	TIP	S	293	91.680	69.354	38.601	1.00	85.69
ATOM	5529	OH2	TIP	S	294	28.082	41.729	32.923	1.00	66.85
ATOM	5530	OH2	TIP	S	295	73.741	80.400	18.356	1.00	80.87
ATOM	5531	OH2	TIP	S	296	32.076	32.496	5.281	1.00	73.93
ATOM	5532	OH2	TIP	S	297	91.907	54.059	29.342	1.00	103.71
ATOM	5533	OH2	TIP	S	298	64.727	54.193	7.345	1.00	69.64
TER	5534		TIP	S	298					
ATOM	5535	C1	NAG	N	800	78.925	71.175	49.271	1.00	90.04
ATOM	5536	C2	NAG	N	800	78.492	71.598	50.693	1.00	92.02
ATOM	5537	N2	NAG	N	800	77.567	70.609	51.219	1.00	93.71
ATOM	5538	C7	NAG	N	800	77.690	70.159	52.465	1.00	93.92
ATOM	5539	O7	NAG	N	800	78.362	69.168	52.756	1.00	93.60
ATOM	5540	C8	NAG	N	800	76.942	70.916	53.552	1.00	94.42

Figure 2A-100

[illegible]

201/396

Figure 3A-1

	<u>Atom</u>	<u>Type</u>	<u>Resid</u>	<u>#</u>	<u>X</u>	<u>Y</u>	<u>Z</u>	<u>Occ</u>	<u>B</u>	
ATOM	1	N	SER A	19	2.776	21.441	1.520	1.00	97.78	N
ATOM	2	CA	SER A	19	3.974	21.011	0.719	1.00	97.77	C
ATOM	3	CB	SER A	19	5.237	21.748	1.189	1.00	97.91	C
ATOM	4	OG	SER A	19	4.949	23.087	1.573	1.00	98.18	O
ATOM	5	C	SER A	19	4.189	19.493	0.764	1.00	97.47	C
ATOM	6	O	SER A	19	3.646	18.814	1.648	1.00	97.51	O
ATOM	7	N	THR A	20	4.988	18.979	-0.178	1.00	96.98	N
ATOM	8	CA	THR A	20	5.226	17.532	-0.351	1.00	96.65	C
ATOM	9	CB	THR A	20	6.261	17.308	-1.466	1.00	96.78	C
ATOM	10	OG1	THR A	20	6.342	18.488	-2.286	1.00	96.86	O
ATOM	11	CG2	THR A	20	5.793	16.201	-2.425	1.00	97.17	C
ATOM	12	C	THR A	20	5.617	16.747	0.925	1.00	96.12	C
ATOM	13	O	THR A	20	5.607	17.292	2.027	1.00	96.22	O
ATOM	14	N	ILE A	21	5.944	15.465	0.778	1.00	95.42	N
ATOM	15	CA	ILE A	21	6.257	14.602	1.936	1.00	94.62	C
ATOM	16	CB	ILE A	21	5.676	13.152	1.731	1.00	94.76	C
ATOM	17	CG1	ILE A	21	4.305	13.199	1.042	1.00	95.22	C
ATOM	18	CD1	ILE A	21	4.295	12.648	-0.383	1.00	96.01	C
ATOM	19	CG2	ILE A	21	5.526	12.407	3.053	1.00	94.54	C
ATOM	20	C	ILE A	21	7.754	14.596	2.351	1.00	93.79	C
ATOM	21	O	ILE A	21	8.098	14.239	3.472	1.00	93.39	O
ATOM	22	N	GLU A	22	8.631	15.010	1.445	1.00	93.00	N
ATOM	23	CA	GLU A	22	10.050	15.143	1.749	1.00	92.25	C
ATOM	24	CB	GLU A	22	10.880	15.147	0.471	1.00	92.90	C
ATOM	25	CG	GLU A	22	11.558	16.481	0.153	1.00	93.67	C
ATOM	26	CD	GLU A	22	13.057	16.336	0.042	1.00	94.67	C
ATOM	27	OE1	GLU A	22	13.545	15.226	0.391	1.00	94.66	O
ATOM	28	OE2	GLU A	22	13.730	17.317	-0.392	1.00	94.25	O
ATOM	29	C	GLU A	22	10.292	16.433	2.475	1.00	91.31	C
ATOM	30	O	GLU A	22	11.296	16.571	3.168	1.00	91.35	O
ATOM	31	N	GLU A	23	9.397	17.394	2.259	1.00	90.13	N
ATOM	32	CA	GLU A	23	9.293	18.555	3.126	1.00	89.05	C
ATOM	33	CB	GLU A	23	8.386	19.600	2.498	1.00	89.10	C
ATOM	34	CG	GLU A	23	7.866	20.627	3.481	1.00	88.64	C
ATOM	35	CD	GLU A	23	8.979	21.255	4.283	1.00	88.52	C
ATOM	36	OE1	GLU A	23	8.923	21.171	5.530	1.00	88.66	O
ATOM	37	OE2	GLU A	23	9.909	21.814	3.660	1.00	88.48	O
ATOM	38	C	GLU A	23	8.722	18.124	4.472	1.00	88.38	C
ATOM	39	O	GLU A	23	9.097	18.658	5.510	1.00	87.69	O
ATOM	40	N	GLN A	24	7.818	17.142	4.430	1.00	88.09	N
ATOM	41	CA	GLN A	24	7.164	16.570	5.627	1.00	87.86	C
ATOM	42	CB	GLN A	24	6.132	15.467	5.230	1.00	88.17	C
ATOM	43	CG	GLN A	24	4.677	16.007	4.947	1.00	89.99	C
ATOM	44	CD	GLN A	24	3.877	15.232	3.875	1.00	90.67	C
ATOM	45	OE1	GLN A	24	3.610	14.038	4.044	1.00	91.59	O
ATOM	46	NE2	GLN A	24	3.474	15.920	2.796	1.00	88.58	N
ATOM	47	C	GLN A	24	8.168	16.080	6.704	1.00	86.81	C
ATOM	48	O	GLN A	24	7.920	16.202	7.913	1.00	86.79	O
ATOM	49	N	ALA A	25	9.296	15.544	6.235	1.00	85.41	N
ATOM	50	CA	ALA A	25	10.417	15.147	7.068	1.00	83.62	C
ATOM	51	CB	ALA A	25	11.479	14.499	6.215	1.00	83.71	C
ATOM	52	C	ALA A	25	10.995	16.352	7.781	1.00	82.61	C
ATOM	53	O	ALA A	25	10.866	16.471	8.999	1.00	82.28	O

202/396

Figure 3A-2

ATOM	54	N	LYS	A	26	11.609	17.249	7.012	1.00	81.31	N
ATOM	55	CA	LYS	A	26	12.363	18.389	7.547	1.00	80.69	C
ATOM	56	CB	LYS	A	26	12.374	19.536	6.534	1.00	80.57	C
ATOM	57	CG	LYS	A	26	13.490	19.430	5.501	1.00	80.85	C
ATOM	58	CD	LYS	A	26	12.982	19.014	4.127	1.00	80.39	C
ATOM	59	CE	LYS	A	26	13.461	19.965	3.028	1.00	80.17	C
ATOM	60	NZ	LYS	A	26	12.413	20.204	1.976	1.00	80.34	N
ATOM	61	C	LYS	A	26	12.026	18.922	8.970	1.00	80.27	C
ATOM	62	O	LYS	A	26	12.943	19.341	9.684	1.00	80.42	O
ATOM	63	N	THR	A	27	10.743	18.911	9.369	1.00	79.61	N
ATOM	64	CA	THR	A	27	10.314	19.395	10.699	1.00	78.76	C
ATOM	65	CB	THR	A	27	8.849	19.977	10.718	1.00	79.12	C
ATOM	66	OG1	THR	A	27	8.748	21.009	11.719	1.00	79.27	O
ATOM	67	CG2	THR	A	27	7.812	18.928	11.216	1.00	78.71	C
ATOM	68	C	THR	A	27	10.414	18.324	11.753	1.00	77.96	C
ATOM	69	O	THR	A	27	10.693	18.617	12.921	1.00	78.09	O
ATOM	70	N	PHE	A	28	10.150	17.085	11.353	1.00	76.71	N
ATOM	71	CA	PHE	A	28	10.089	16.007	12.327	1.00	75.37	C
ATOM	72	CB	PHE	A	28	9.585	14.732	11.716	1.00	74.88	C
ATOM	73	CG	PHE	A	28	9.460	13.683	12.693	1.00	73.56	C
ATOM	74	CD1	PHE	A	28	8.826	13.951	13.893	1.00	73.49	C
ATOM	75	CE1	PHE	A	28	8.711	12.997	14.855	1.00	74.91	C
ATOM	76	CZ	PHE	A	28	9.267	11.749	14.630	1.00	75.46	C
ATOM	77	CE2	PHE	A	28	9.937	11.483	13.418	1.00	75.20	C
ATOM	78	CD2	PHE	A	28	10.033	12.456	12.473	1.00	74.06	C
ATOM	79	C	PHE	A	28	11.446	15.776	12.998	1.00	74.85	C
ATOM	80	O	PHE	A	28	11.523	15.527	14.222	1.00	75.14	O
ATOM	81	N	LEU	A	29	12.493	15.832	12.163	1.00	73.39	N
ATOM	82	CA	LEU	A	29	13.827	16.248	12.576	1.00	71.24	C
ATOM	83	CB	LEU	A	29	14.606	16.809	11.379	1.00	70.92	C
ATOM	84	CG	LEU	A	29	15.529	15.994	10.489	1.00	69.34	C
ATOM	85	CD1	LEU	A	29	14.836	14.725	9.980	1.00	67.44	C
ATOM	86	CD2	LEU	A	29	15.992	16.895	9.351	1.00	67.18	C
ATOM	87	C	LEU	A	29	13.637	17.394	13.542	1.00	70.20	C
ATOM	88	O	LEU	A	29	13.762	17.218	14.738	1.00	69.81	O
ATOM	89	N	ASP	A	30	13.283	18.556	13.000	1.00	68.92	N
ATOM	90	CA	ASP	A	30	13.404	19.811	13.718	1.00	68.01	C
ATOM	91	CB	ASP	A	30	12.931	20.983	12.886	1.00	68.39	C
ATOM	92	CG	ASP	A	30	13.884	22.122	12.966	1.00	69.71	C
ATOM	93	OD1	ASP	A	30	15.042	21.836	13.336	1.00	71.67	O
ATOM	94	OD2	ASP	A	30	13.594	23.314	12.712	1.00	71.01	O
ATOM	95	C	ASP	A	30	12.765	19.857	15.074	1.00	66.95	C
ATOM	96	O	ASP	A	30	13.145	20.665	15.901	1.00	66.60	O
ATOM	97	N	LYS	A	31	11.787	18.992	15.286	1.00	66.08	N
ATOM	98	CA	LYS	A	31	11.313	18.687	16.621	1.00	65.49	C
ATOM	99	CB	LYS	A	31	9.802	18.443	16.611	1.00	65.44	C
ATOM	100	CG	LYS	A	31	8.946	19.559	17.239	1.00	63.40	C
ATOM	101	CD	LYS	A	31	7.729	19.014	18.018	1.00	60.25	C
ATOM	102	CE	LYS	A	31	6.881	18.058	17.195	1.00	58.67	C
ATOM	103	NZ	LYS	A	31	6.528	16.783	17.897	1.00	58.17	N
ATOM	104	C	LYS	A	31	12.126	17.436	17.016	1.00	65.68	C
ATOM	105	O	LYS	A	31	11.613	16.316	17.270	1.00	65.79	O
ATOM	106	N	PHE	A	32	13.433	17.648	16.984	1.00	65.01	N
ATOM	107	CA	PHE	A	32	14.405	16.649	17.339	1.00	64.09	C
ATOM	108	CB	PHE	A	32	14.718	15.705	16.185	1.00	64.07	C
ATOM	109	CG	PHE	A	32	15.235	14.405	16.641	1.00	65.35	C

203/396

Figure 3A-3

ATOM	110	CD1	PHE	A	32	16.609	14.186	16.742	1.00	64.99	C
ATOM	111	CE1	PHE	A	32	17.104	12.970	17.211	1.00	64.89	C
ATOM	112	CZ	PHE	A	32	16.224	11.963	17.593	1.00	65.88	C
ATOM	113	CE2	PHE	A	32	14.838	12.180	17.516	1.00	66.47	C
ATOM	114	CD2	PHE	A	32	14.353	13.402	17.045	1.00	66.33	C
ATOM	115	C	PHE	A	32	15.598	17.468	17.675	1.00	63.18	C
ATOM	116	O	PHE	A	32	15.813	17.787	18.844	1.00	63.31	O
ATOM	117	N	ASN	A	33	16.334	17.866	16.647	1.00	62.03	N
ATOM	118	CA	ASN	A	33	17.496	18.735	16.810	1.00	61.68	C
ATOM	119	CB	ASN	A	33	17.701	19.611	15.569	1.00	61.73	C
ATOM	120	CG	ASN	A	33	17.792	18.804	14.274	1.00	63.34	C
ATOM	121	OD1	ASN	A	33	17.930	19.382	13.187	1.00	64.46	O
ATOM	122	ND2	ASN	A	33	17.713	17.463	14.376	1.00	65.00	N
ATOM	123	C	ASN	A	33	17.405	19.642	18.034	1.00	61.17	C
ATOM	124	O	ASN	A	33	18.395	20.259	18.445	1.00	61.39	O
ATOM	125	N	HIS	A	34	16.217	19.704	18.626	1.00	60.28	N
ATOM	126	CA	HIS	A	34	15.892	20.792	19.504	1.00	59.21	C
ATOM	127	CB	HIS	A	34	14.963	21.736	18.778	1.00	58.62	C
ATOM	128	CG	HIS	A	34	15.680	22.812	18.035	1.00	57.00	C
ATOM	129	ND1	HIS	A	34	16.461	23.756	18.669	1.00	57.18	N
ATOM	130	CE1	HIS	A	34	16.959	24.589	17.774	1.00	55.63	C
ATOM	131	NE2	HIS	A	34	16.532	24.220	16.582	1.00	55.86	N
ATOM	132	CD2	HIS	A	34	15.738	23.102	16.716	1.00	55.52	C
ATOM	133	C	HIS	A	34	15.296	20.346	20.798	1.00	59.33	C
ATOM	134	O	HIS	A	34	15.608	20.922	21.838	1.00	58.83	O
ATOM	135	N	GLU	A	35	14.438	19.335	20.746	1.00	59.88	N
ATOM	136	CA	GLU	A	35	13.892	18.806	21.989	1.00	61.52	C
ATOM	137	CB	GLU	A	35	12.534	18.109	21.792	1.00	61.61	C
ATOM	138	CG	GLU	A	35	11.637	18.163	23.039	1.00	63.17	C
ATOM	139	CD	GLU	A	35	10.923	16.846	23.377	1.00	66.05	C
ATOM	140	OE1	GLU	A	35	11.157	15.830	22.656	1.00	67.96	O
ATOM	141	OE2	GLU	A	35	10.116	16.824	24.361	1.00	64.84	O
ATOM	142	C	GLU	A	35	14.909	17.846	22.602	1.00	62.46	C
ATOM	143	O	GLU	A	35	15.350	18.019	23.760	1.00	62.76	O
ATOM	144	N	ALA	A	36	15.264	16.834	21.801	1.00	63.26	N
ATOM	145	CA	ALA	A	36	16.286	15.853	22.123	1.00	63.16	C
ATOM	146	CB	ALA	A	36	16.516	14.931	20.934	1.00	63.07	C
ATOM	147	C	ALA	A	36	17.576	16.561	22.547	1.00	63.47	C
ATOM	148	O	ALA	A	36	18.047	16.330	23.668	1.00	63.60	O
ATOM	149	N	GLU	A	37	18.121	17.444	21.695	1.00	63.14	N
ATOM	150	CA	GLU	A	37	19.326	18.183	22.075	1.00	63.24	C
ATOM	151	CB	GLU	A	37	19.390	19.586	21.441	1.00	63.88	C
ATOM	152	CG	GLU	A	37	20.397	20.560	22.099	1.00	66.10	C
ATOM	153	CD	GLU	A	37	21.096	21.525	21.123	1.00	67.99	C
ATOM	154	OE1	GLU	A	37	20.777	21.514	19.901	1.00	68.06	O
ATOM	155	OE2	GLU	A	37	21.969	22.310	21.588	1.00	67.48	O
ATOM	156	C	GLU	A	37	19.370	18.276	23.588	1.00	62.47	C
ATOM	157	O	GLU	A	37	20.185	17.643	24.217	1.00	62.48	O
ATOM	158	N	ASP	A	38	18.444	19.014	24.170	1.00	62.03	N
ATOM	159	CA	ASP	A	38	18.467	19.260	25.599	1.00	62.13	C
ATOM	160	CB	ASP	A	38	17.744	20.576	25.920	1.00	63.22	C
ATOM	161	CG	ASP	A	38	17.313	20.680	27.378	1.00	66.31	C
ATOM	162	OD1	ASP	A	38	18.195	20.866	28.265	1.00	69.30	O
ATOM	163	OD2	ASP	A	38	16.107	20.594	27.725	1.00	69.78	O
ATOM	164	C	ASP	A	38	17.908	18.095	26.402	1.00	60.85	C
ATOM	165	O	ASP	A	38	18.245	17.921	27.579	1.00	60.41	O

204/396

Figure 3A-4

ATOM	166	N	LEU	A	39	17.068	17.283	25.767	1.00	59.76	N
ATOM	167	CA	LEU	A	39	16.700	16.005	26.390	1.00	58.46	C
ATOM	168	CB	LEU	A	39	15.278	15.519	26.040	1.00	57.94	C
ATOM	169	CG	LEU	A	39	14.637	14.906	27.298	1.00	56.33	C
ATOM	170	CD1	LEU	A	39	14.631	13.390	27.216	1.00	55.31	C
ATOM	171	CD2	LEU	A	39	15.331	15.358	28.622	1.00	54.73	C
ATOM	172	C	LEU	A	39	17.790	14.926	26.216	1.00	57.55	C
ATOM	173	O	LEU	A	39	17.679	13.803	26.745	1.00	57.58	O
ATOM	174	N	PHE	A	40	18.844	15.281	25.486	1.00	55.99	N
ATOM	175	CA	PHE	A	40	20.120	14.625	25.691	1.00	54.86	C
ATOM	176	CB	PHE	A	40	21.095	14.917	24.548	1.00	54.83	C
ATOM	177	CG	PHE	A	40	22.353	14.083	24.590	1.00	54.87	C
ATOM	178	CD1	PHE	A	40	22.337	12.783	25.100	1.00	55.39	C
ATOM	179	CE1	PHE	A	40	23.482	12.024	25.129	1.00	54.81	C
ATOM	180	CZ	PHE	A	40	24.661	12.549	24.629	1.00	54.32	C
ATOM	181	CE2	PHE	A	40	24.688	13.822	24.115	1.00	53.93	C
ATOM	182	CD2	PHE	A	40	23.544	14.585	24.104	1.00	54.42	C
ATOM	183	C	PHE	A	40	20.654	15.206	26.981	1.00	53.78	C
ATOM	184	O	PHE	A	40	20.610	14.582	28.035	1.00	53.06	O
ATOM	185	N	TYR	A	41	21.092	16.450	26.865	1.00	52.95	N
ATOM	186	CA	TYR	A	41	21.682	17.228	27.940	1.00	52.17	C
ATOM	187	CB	TYR	A	41	21.768	18.690	27.519	1.00	51.05	C
ATOM	188	CG	TYR	A	41	22.482	19.522	28.509	1.00	49.64	C
ATOM	189	CD1	TYR	A	41	23.546	20.320	28.138	1.00	50.09	C
ATOM	190	CE1	TYR	A	41	24.204	21.098	29.083	1.00	50.14	C
ATOM	191	CZ	TYR	A	41	23.781	21.051	30.405	1.00	50.22	C
ATOM	192	OH	TYR	A	41	24.384	21.802	31.376	1.00	52.93	O
ATOM	193	CE2	TYR	A	41	22.732	20.263	30.782	1.00	48.99	C
ATOM	194	CD2	TYR	A	41	22.092	19.518	29.839	1.00	48.77	C
ATOM	195	C	TYR	A	41	21.055	17.083	29.345	1.00	52.52	C
ATOM	196	O	TYR	A	41	21.653	17.473	30.355	1.00	52.45	O
ATOM	197	N	GLN	A	42	19.881	16.502	29.473	1.00	52.75	N
ATOM	198	CA	GLN	A	42	19.485	16.338	30.849	1.00	53.41	C
ATOM	199	CB	GLN	A	42	18.010	16.674	31.084	1.00	53.91	C
ATOM	200	CG	GLN	A	42	17.830	18.065	31.810	1.00	54.41	C
ATOM	201	CD	GLN	A	42	18.005	19.322	30.893	1.00	53.22	C
ATOM	202	OE1	GLN	A	42	17.914	20.461	31.366	1.00	51.57	O
ATOM	203	NE2	GLN	A	42	18.255	19.098	29.605	1.00	52.65	N
ATOM	204	C	GLN	A	42	19.971	15.016	31.410	1.00	53.58	C
ATOM	205	O	GLN	A	42	20.321	14.923	32.585	1.00	53.71	O
ATOM	206	N	SER	A	43	20.019	14.007	30.545	1.00	53.65	N
ATOM	207	CA	SER	A	43	20.773	12.776	30.790	1.00	53.50	C
ATOM	208	CB	SER	A	43	20.458	11.741	29.693	1.00	53.62	C
ATOM	209	OG	SER	A	43	19.830	10.574	30.198	1.00	53.32	O
ATOM	210	C	SER	A	43	22.310	13.063	30.828	1.00	53.35	C
ATOM	211	O	SER	A	43	22.990	12.730	31.817	1.00	53.77	O
ATOM	212	N	SER	A	44	22.850	13.685	29.767	1.00	52.22	N
ATOM	213	CA	SER	A	44	24.288	13.984	29.677	1.00	50.74	C
ATOM	214	CB	SER	A	44	24.606	14.934	28.506	1.00	50.56	C
ATOM	215	OG	SER	A	44	25.110	14.253	27.358	1.00	48.72	O
ATOM	216	C	SER	A	44	24.837	14.528	31.003	1.00	50.03	C
ATOM	217	O	SER	A	44	26.034	14.442	31.282	1.00	50.30	O
ATOM	218	N	LEU	A	45	23.962	15.044	31.847	1.00	48.88	N
ATOM	219	CA	LEU	A	45	24.441	15.529	33.114	1.00	48.19	C
ATOM	220	CB	LEU	A	45	23.962	16.951	33.382	1.00	48.92	C
ATOM	221	CG	LEU	A	45	25.095	17.969	33.606	1.00	50.24	C

205/396

Figure 3A-5

ATOM	222	CD1	LEU	A	45	24.495	19.383	33.666	1.00	51.70	C
ATOM	223	CD2	LEU	A	45	25.979	17.654	34.867	1.00	51.17	C
ATOM	224	C	LEU	A	45	24.134	14.626	34.266	1.00	46.95	C
ATOM	225	O	LEU	A	45	24.903	14.567	35.191	1.00	47.01	O
ATOM	226	N	ALA	A	46	23.025	13.915	34.219	1.00	46.04	N
ATOM	227	CA	ALA	A	46	22.783	12.875	35.208	1.00	45.88	C
ATOM	228	CB	ALA	A	46	21.664	11.944	34.765	1.00	46.08	C
ATOM	229	C	ALA	A	46	24.039	12.090	35.258	1.00	45.79	C
ATOM	230	O	ALA	A	46	24.529	11.734	36.326	1.00	45.75	O
ATOM	231	N	SER	A	47	24.542	11.828	34.055	1.00	45.88	N
ATOM	232	CA	SER	A	47	25.662	10.953	33.821	1.00	45.58	C
ATOM	233	CB	SER	A	47	25.836	10.715	32.329	1.00	45.52	C
ATOM	234	OG	SER	A	47	25.678	9.343	32.043	1.00	45.41	O
ATOM	235	C	SER	A	47	26.887	11.575	34.439	1.00	45.66	C
ATOM	236	O	SER	A	47	27.325	11.114	35.481	1.00	46.08	O
ATOM	237	N	TRP	A	48	27.424	12.635	33.853	1.00	45.12	N
ATOM	238	CA	TRP	A	48	28.586	13.233	34.447	1.00	45.16	C
ATOM	239	CB	TRP	A	48	28.506	14.716	34.359	1.00	45.70	C
ATOM	240	CG	TRP	A	48	29.791	15.356	34.742	1.00	47.93	C
ATOM	241	CD1	TRP	A	48	30.077	15.996	35.910	1.00	50.19	C
ATOM	242	NE1	TRP	A	48	31.368	16.468	35.892	1.00	50.30	N
ATOM	243	CE2	TRP	A	48	31.934	16.132	34.695	1.00	49.54	C
ATOM	244	CD2	TRP	A	48	30.972	15.418	33.957	1.00	48.40	C
ATOM	245	CE3	TRP	A	48	31.313	14.950	32.699	1.00	48.24	C
ATOM	246	CZ3	TRP	A	48	32.559	15.200	32.227	1.00	51.03	C
ATOM	247	CH2	TRP	A	48	33.497	15.918	32.979	1.00	51.47	C
ATOM	248	CZ2	TRP	A	48	33.197	16.393	34.213	1.00	50.74	C
ATOM	249	C	TRP	A	48	28.563	12.924	35.891	1.00	44.84	C
ATOM	250	O	TRP	A	48	29.235	12.034	36.367	1.00	44.53	O
ATOM	251	N	ASN	A	49	27.764	13.692	36.591	1.00	45.29	N
ATOM	252	CA	ASN	A	49	27.533	13.483	37.997	1.00	46.78	C
ATOM	253	CB	ASN	A	49	26.068	13.744	38.288	1.00	46.73	C
ATOM	254	CG	ASN	A	49	25.861	15.062	38.933	1.00	47.30	C
ATOM	255	OD1	ASN	A	49	25.670	15.105	40.134	1.00	48.18	O
ATOM	256	ND2	ASN	A	49	25.950	16.168	38.155	1.00	47.09	N
ATOM	257	C	ASN	A	49	27.940	12.125	38.552	1.00	47.68	C
ATOM	258	O	ASN	A	49	28.785	12.035	39.452	1.00	47.95	O
ATOM	259	N	TYR	A	50	27.324	11.073	38.015	1.00	48.91	N
ATOM	260	CA	TYR	A	50	27.564	9.693	38.459	1.00	49.64	C
ATOM	261	CB	TYR	A	50	26.595	8.741	37.780	1.00	49.13	C
ATOM	262	CG	TYR	A	50	26.946	7.303	37.974	1.00	48.32	C
ATOM	263	CD1	TYR	A	50	26.715	6.670	39.184	1.00	49.31	C
ATOM	264	CE1	TYR	A	50	27.024	5.349	39.367	1.00	51.51	C
ATOM	265	CZ	TYR	A	50	27.580	4.639	38.311	1.00	53.42	C
ATOM	266	OH	TYR	A	50	27.907	3.288	38.444	1.00	55.26	O
ATOM	267	CE2	TYR	A	50	27.822	5.276	37.102	1.00	51.12	C
ATOM	268	CD2	TYR	A	50	27.512	6.588	36.955	1.00	48.33	C
ATOM	269	C	TYR	A	50	28.995	9.224	38.192	1.00	50.39	C
ATOM	270	O	TYR	A	50	29.623	8.565	39.044	1.00	50.78	O
ATOM	271	N	ASN	A	51	29.494	9.547	37.001	1.00	50.61	N
ATOM	272	CA	ASN	A	51	30.868	9.250	36.683	1.00	50.56	C
ATOM	273	CB	ASN	A	51	31.108	9.275	35.186	1.00	49.97	C
ATOM	274	CG	ASN	A	51	29.940	8.800	34.407	1.00	48.18	C
ATOM	275	OD1	ASN	A	51	29.306	9.592	33.740	1.00	46.64	O
ATOM	276	ND2	ASN	A	51	29.656	7.499	34.454	1.00	46.55	N
ATOM	277	C	ASN	A	51	31.811	10.206	37.366	1.00	51.30	C

206/396

Figure 3A-6

ATOM	278	O	ASN	A	51	33.010	9.990	37.348	1.00	51.77	O
ATOM	279	N	THR	A	52	31.296	11.272	37.956	1.00	52.18	N
ATOM	280	CA	THR	A	52	32.175	12.102	38.748	1.00	53.65	C
ATOM	281	CB	THR	A	52	32.102	13.598	38.409	1.00	53.65	C
ATOM	282	OG1	THR	A	52	31.381	13.827	37.198	1.00	53.75	O
ATOM	283	CG2	THR	A	52	33.482	14.088	38.098	1.00	54.13	C
ATOM	284	C	THR	A	52	31.921	11.926	40.217	1.00	54.79	C
ATOM	285	O	THR	A	52	32.621	12.509	41.029	1.00	55.16	O
ATOM	286	N	ASN	A	53	30.918	11.141	40.573	1.00	56.19	N
ATOM	287	CA	ASN	A	53	30.662	10.881	41.977	1.00	57.87	C
ATOM	288	CB	ASN	A	53	30.039	12.103	42.662	1.00	58.21	C
ATOM	289	CG	ASN	A	53	29.949	11.946	44.184	1.00	59.60	C
ATOM	290	OD1	ASN	A	53	29.336	12.774	44.864	1.00	61.34	O
ATOM	291	ND2	ASN	A	53	30.564	10.886	44.723	1.00	60.98	N
ATOM	292	C	ASN	A	53	29.741	9.717	42.110	1.00	58.61	C
ATOM	293	O	ASN	A	53	28.601	9.808	41.689	1.00	58.57	O
ATOM	294	N	ILE	A	54	30.225	8.627	42.692	1.00	59.97	N
ATOM	295	CA	ILE	A	54	29.355	7.481	42.867	1.00	61.88	C
ATOM	296	CB	ILE	A	54	30.035	6.129	42.544	1.00	61.70	C
ATOM	297	CG1	ILE	A	54	30.461	6.083	41.083	1.00	61.23	C
ATOM	298	CD1	ILE	A	54	31.835	5.474	40.889	1.00	60.75	C
ATOM	299	CG2	ILE	A	54	29.072	4.953	42.825	1.00	61.77	C
ATOM	300	C	ILE	A	54	28.687	7.478	44.238	1.00	63.46	C
ATOM	301	O	ILE	A	54	29.322	7.281	45.283	1.00	63.78	O
ATOM	302	N	THR	A	55	27.382	7.721	44.196	1.00	65.13	N
ATOM	303	CA	THR	A	55	26.509	7.527	45.331	1.00	66.70	C
ATOM	304	CB	THR	A	55	25.894	8.904	45.752	1.00	66.72	C
ATOM	305	OG1	THR	A	55	26.877	9.934	45.565	1.00	66.35	O
ATOM	306	CG2	THR	A	55	25.561	8.973	47.288	1.00	66.29	C
ATOM	307	C	THR	A	55	25.467	6.465	44.910	1.00	67.79	C
ATOM	308	O	THR	A	55	25.822	5.430	44.334	1.00	67.97	O
ATOM	309	N	GLU	A	56	24.209	6.711	45.258	1.00	69.19	N
ATOM	310	CA	GLU	A	56	23.048	6.066	44.669	1.00	70.53	C
ATOM	311	CB	GLU	A	56	22.715	4.758	45.374	1.00	70.95	C
ATOM	312	CG	GLU	A	56	22.802	3.551	44.440	1.00	73.87	C
ATOM	313	CD	GLU	A	56	21.449	3.130	43.856	1.00	77.46	C
ATOM	314	OE1	GLU	A	56	20.419	3.793	44.167	1.00	78.52	O
ATOM	315	OE2	GLU	A	56	21.411	2.126	43.086	1.00	78.64	O
ATOM	316	C	GLU	A	56	21.934	7.107	44.769	1.00	70.73	C
ATOM	317	O	GLU	A	56	20.735	6.825	44.650	1.00	70.91	O
ATOM	318	N	GLU	A	57	22.385	8.328	45.025	1.00	71.06	N
ATOM	319	CA	GLU	A	57	21.639	9.529	44.736	1.00	71.64	C
ATOM	320	CB	GLU	A	57	22.174	10.694	45.573	1.00	71.71	C
ATOM	321	CG	GLU	A	57	21.774	10.610	47.040	1.00	73.49	C
ATOM	322	CD	GLU	A	57	21.089	9.293	47.388	1.00	74.79	C
ATOM	323	OE1	GLU	A	57	19.848	9.294	47.579	1.00	74.44	O
ATOM	324	OE2	GLU	A	57	21.797	8.256	47.455	1.00	75.18	O
ATOM	325	C	GLU	A	57	21.833	9.808	43.260	1.00	71.64	C
ATOM	326	O	GLU	A	57	21.130	10.621	42.672	1.00	72.10	O
ATOM	327	N	ASN	A	58	22.780	9.106	42.656	1.00	71.30	N
ATOM	328	CA	ASN	A	58	23.189	9.438	41.322	1.00	71.02	C
ATOM	329	CB	ASN	A	58	24.603	9.960	41.353	1.00	70.74	C
ATOM	330	CG	ASN	A	58	24.705	11.233	42.148	1.00	70.71	C
ATOM	331	OD1	ASN	A	58	24.553	11.243	43.374	1.00	69.55	O
ATOM	332	ND2	ASN	A	58	24.921	12.332	41.450	1.00	72.02	N
ATOM	333	C	ASN	A	58	23.017	8.310	40.353	1.00	71.26	C

207/396

Figure 3A-7

ATOM	334	O	ASN	A	58	22.700	8.557	39.201	1.00	71.32	O
ATOM	335	N	VAL	A	59	23.199	7.073	40.811	1.00	71.68	N
ATOM	336	CA	VAL	A	59	22.874	5.914	39.978	1.00	72.27	C
ATOM	337	CB	VAL	A	59	22.967	4.570	40.738	1.00	72.33	C
ATOM	338	CG1	VAL	A	59	22.069	3.501	40.057	1.00	71.83	C
ATOM	339	CG2	VAL	A	59	24.430	4.092	40.887	1.00	72.19	C
ATOM	340	C	VAL	A	59	21.429	6.096	39.558	1.00	72.86	C
ATOM	341	O	VAL	A	59	21.113	6.165	38.366	1.00	73.19	O
ATOM	342	N	GLN	A	60	20.569	6.209	40.573	1.00	73.34	N
ATOM	343	CA	GLN	A	60	19.144	6.474	40.415	1.00	73.30	C
ATOM	344	CB	GLN	A	60	18.454	6.556	41.790	1.00	73.23	C
ATOM	345	CG	GLN	A	60	17.535	5.372	42.058	1.00	73.21	C
ATOM	346	CD	GLN	A	60	17.239	4.583	40.785	1.00	74.01	C
ATOM	347	OE1	GLN	A	60	16.507	5.060	39.907	1.00	74.03	O
ATOM	348	NE2	GLN	A	60	17.827	3.387	40.670	1.00	74.32	N
ATOM	349	C	GLN	A	60	18.860	7.706	39.546	1.00	73.25	C
ATOM	350	O	GLN	A	60	18.252	7.576	38.481	1.00	73.38	O
ATOM	351	N	ASN	A	61	19.331	8.875	39.984	1.00	72.98	N
ATOM	352	CA	ASN	A	61	19.180	10.120	39.235	1.00	72.98	C
ATOM	353	CB	ASN	A	61	20.009	11.203	39.884	1.00	73.34	C
ATOM	354	CG	ASN	A	61	19.230	11.975	40.896	1.00	75.39	C
ATOM	355	OD1	ASN	A	61	19.270	13.215	40.917	1.00	77.08	O
ATOM	356	ND2	ASN	A	61	18.498	11.252	41.759	1.00	77.46	N
ATOM	357	C	ASN	A	61	19.587	10.054	37.785	1.00	72.46	C
ATOM	358	O	ASN	A	61	18.975	10.692	36.932	1.00	72.33	O
ATOM	359	N	MET	A	62	20.648	9.298	37.537	1.00	72.05	N
ATOM	360	CA	MET	A	62	21.189	9.096	36.210	1.00	71.71	C
ATOM	361	CB	MET	A	62	22.533	8.375	36.315	1.00	71.50	C
ATOM	362	CG	MET	A	62	23.506	8.624	35.165	1.00	69.69	C
ATOM	363	SD	MET	A	62	24.208	7.104	34.519	1.00	65.75	S
ATOM	364	CE	MET	A	62	23.970	5.904	35.930	1.00	63.09	C
ATOM	365	C	MET	A	62	20.218	8.295	35.342	1.00	72.08	C
ATOM	366	O	MET	A	62	19.813	8.768	34.270	1.00	72.24	O
ATOM	367	N	ASN	A	63	19.847	7.091	35.802	1.00	71.96	N
ATOM	368	CA	ASN	A	63	18.929	6.227	35.044	1.00	71.78	C
ATOM	369	CB	ASN	A	63	19.241	4.704	35.217	1.00	71.93	C
ATOM	370	CG	ASN	A	63	18.906	4.129	36.623	1.00	71.76	C
ATOM	371	OD1	ASN	A	63	18.343	4.808	37.496	1.00	71.41	O
ATOM	372	ND2	ASN	A	63	19.261	2.846	36.824	1.00	70.15	N
ATOM	373	C	ASN	A	63	17.430	6.633	35.158	1.00	71.60	C
ATOM	374	O	ASN	A	63	16.540	6.003	34.565	1.00	71.69	O
ATOM	375	N	ASN	A	64	17.172	7.705	35.909	1.00	71.08	N
ATOM	376	CA	ASN	A	64	15.917	8.439	35.797	1.00	70.32	C
ATOM	377	CB	ASN	A	64	15.559	9.201	37.084	1.00	70.19	C
ATOM	378	CG	ASN	A	64	14.932	8.310	38.147	1.00	69.54	C
ATOM	379	OD1	ASN	A	64	14.747	7.107	37.950	1.00	67.14	O
ATOM	380	ND2	ASN	A	64	14.622	8.906	39.297	1.00	69.55	N
ATOM	381	C	ASN	A	64	16.024	9.411	34.634	1.00	69.89	C
ATOM	382	O	ASN	A	64	15.174	9.401	33.759	1.00	69.99	O
ATOM	383	N	ALA	A	65	17.072	10.232	34.606	1.00	69.28	N
ATOM	384	CA	ALA	A	65	17.149	11.311	33.619	1.00	68.90	C
ATOM	385	CB	ALA	A	65	18.039	12.455	34.108	1.00	68.97	C
ATOM	386	C	ALA	A	65	17.566	10.823	32.239	1.00	68.62	C
ATOM	387	O	ALA	A	65	18.002	11.610	31.401	1.00	68.15	O
ATOM	388	N	GLY	A	66	17.403	9.518	32.025	1.00	68.69	N
ATOM	389	CA	GLY	A	66	17.623	8.863	30.739	1.00	69.17	C

208/396

Figure 3A-8

ATOM	390	C	GLY	A	66	16.519	7.873	30.348	1.00	69.54	C
ATOM	391	O	GLY	A	66	16.258	7.665	29.147	1.00	69.44	O
ATOM	392	N	ASP	A	67	15.898	7.239	31.357	1.00	69.48	N
ATOM	393	CA	ASP	A	67	14.610	6.549	31.201	1.00	69.15	C
ATOM	394	CB	ASP	A	67	14.058	6.153	32.573	1.00	69.15	C
ATOM	395	CG	ASP	A	67	13.604	4.704	32.627	1.00	70.87	C
ATOM	396	OD1	ASP	A	67	12.794	4.336	31.745	1.00	72.14	O
ATOM	397	OD2	ASP	A	67	13.988	3.864	33.500	1.00	71.71	O
ATOM	398	C	ASP	A	67	13.597	7.433	30.438	1.00	68.66	C
ATOM	399	O	ASP	A	67	12.948	6.972	29.503	1.00	68.80	O
ATOM	400	N	LYS	A	68	13.507	8.705	30.837	1.00	68.06	N
ATOM	401	CA	LYS	A	68	12.720	9.750	30.176	1.00	67.67	C
ATOM	402	CB	LYS	A	68	12.940	11.074	30.929	1.00	67.26	C
ATOM	403	CG	LYS	A	68	11.720	12.002	31.106	1.00	65.94	C
ATOM	404	CD	LYS	A	68	11.128	12.037	32.553	1.00	63.15	C
ATOM	405	CE	LYS	A	68	11.879	12.945	33.559	1.00	60.32	C
ATOM	406	NZ	LYS	A	68	12.240	14.292	33.068	1.00	57.21	N
ATOM	407	C	LYS	A	68	13.153	9.909	28.718	1.00	68.17	C
ATOM	408	O	LYS	A	68	12.434	10.485	27.878	1.00	67.71	O
ATOM	409	N	TRP	A	69	14.346	9.389	28.438	1.00	69.01	N
ATOM	410	CA	TRP	A	69	15.007	9.573	27.147	1.00	69.93	C
ATOM	411	CB	TRP	A	69	16.444	10.115	27.301	1.00	69.44	C
ATOM	412	CG	TRP	A	69	17.207	9.959	26.028	1.00	67.49	C
ATOM	413	CD1	TRP	A	69	17.720	8.806	25.536	1.00	65.97	C
ATOM	414	NE1	TRP	A	69	18.320	9.039	24.324	1.00	65.93	N
ATOM	415	CE2	TRP	A	69	18.190	10.360	24.006	1.00	64.23	C
ATOM	416	CD2	TRP	A	69	17.491	10.971	25.055	1.00	65.15	C
ATOM	417	CE3	TRP	A	69	17.229	12.335	24.966	1.00	64.78	C
ATOM	418	CZ3	TRP	A	69	17.668	13.029	23.851	1.00	64.27	C
ATOM	419	CH2	TRP	A	69	18.364	12.387	22.833	1.00	64.15	C
ATOM	420	CZ2	TRP	A	69	18.629	11.053	22.892	1.00	64.09	C
ATOM	421	C	TRP	A	69	14.985	8.300	26.293	1.00	70.84	C
ATOM	422	O	TRP	A	69	14.851	8.373	25.063	1.00	71.15	O
ATOM	423	N	SER	A	70	15.135	7.139	26.927	1.00	71.72	N
ATOM	424	CA	SER	A	70	14.754	5.891	26.255	1.00	72.47	C
ATOM	425	CB	SER	A	70	15.125	4.647	27.094	1.00	72.67	C
ATOM	426	OG	SER	A	70	16.029	3.808	26.384	1.00	72.98	O
ATOM	427	C	SER	A	70	13.240	5.943	25.897	1.00	72.42	C
ATOM	428	O	SER	A	70	12.872	5.602	24.763	1.00	72.29	O
ATOM	429	N	ALA	A	71	12.410	6.414	26.851	1.00	72.11	N
ATOM	430	CA	ALA	A	71	10.960	6.625	26.683	1.00	71.82	C
ATOM	431	CB	ALA	A	71	10.290	6.974	28.019	1.00	71.47	C
ATOM	432	C	ALA	A	71	10.589	7.653	25.600	1.00	71.79	C
ATOM	433	O	ALA	A	71	9.752	7.348	24.763	1.00	71.72	O
ATOM	434	N	PHE	A	72	11.187	8.854	25.637	1.00	71.84	N
ATOM	435	CA	PHE	A	72	11.129	9.833	24.531	1.00	71.79	C
ATOM	436	CB	PHE	A	72	12.069	11.045	24.831	1.00	71.32	C
ATOM	437	CG	PHE	A	72	12.428	11.974	23.611	1.00	68.61	C
ATOM	438	CD1	PHE	A	72	12.023	11.736	22.317	1.00	65.82	C
ATOM	439	CE1	PHE	A	72	12.387	12.603	21.290	1.00	63.02	C
ATOM	440	CZ	PHE	A	72	13.136	13.707	21.531	1.00	60.97	C
ATOM	441	CE2	PHE	A	72	13.541	13.968	22.773	1.00	62.11	C
ATOM	442	CD2	PHE	A	72	13.200	13.113	23.813	1.00	66.11	C
ATOM	443	C	PHE	A	72	11.481	9.130	23.208	1.00	72.77	C
ATOM	444	O	PHE	A	72	10.604	8.876	22.382	1.00	72.68	O
ATOM	445	N	LEU	A	73	12.756	8.792	23.021	1.00	73.94	N

209/396

Figure 3A-9

ATOM	446	CA	LEU	A	73	13.235	8.281	21.742	1.00	74.88	C
ATOM	447	CB	LEU	A	73	14.699	7.878	21.842	1.00	74.71	C
ATOM	448	CG	LEU	A	73	15.491	8.271	20.599	1.00	74.85	C
ATOM	449	CD1	LEU	A	73	15.431	9.780	20.402	1.00	75.28	C
ATOM	450	CD2	LEU	A	73	16.936	7.758	20.645	1.00	74.67	C
ATOM	451	C	LEU	A	73	12.395	7.122	21.255	1.00	75.72	C
ATOM	452	O	LEU	A	73	12.077	7.024	20.072	1.00	75.34	O
ATOM	453	N	LYS	A	74	12.037	6.260	22.199	1.00	77.27	N
ATOM	454	CA	LYS	A	74	11.082	5.172	21.985	1.00	79.12	C
ATOM	455	CB	LYS	A	74	10.632	4.602	23.345	1.00	79.21	C
ATOM	456	CG	LYS	A	74	9.312	3.840	23.343	1.00	79.45	C
ATOM	457	CD	LYS	A	74	9.490	2.436	22.792	1.00	80.15	C
ATOM	458	CE	LYS	A	74	8.419	2.131	21.781	1.00	80.70	C
ATOM	459	NZ	LYS	A	74	7.140	1.763	22.467	1.00	82.06	N
ATOM	460	C	LYS	A	74	9.853	5.584	21.153	1.00	80.12	C
ATOM	461	O	LYS	A	74	9.525	4.931	20.143	1.00	80.47	O
ATOM	462	N	GLU	A	75	9.177	6.648	21.601	1.00	80.89	N
ATOM	463	CA	GLU	A	75	8.007	7.177	20.912	1.00	81.25	C
ATOM	464	CB	GLU	A	75	7.146	8.055	21.832	1.00	81.41	C
ATOM	465	CG	GLU	A	75	6.321	9.122	21.123	1.00	83.34	C
ATOM	466	CD	GLU	A	75	6.489	10.502	21.749	1.00	86.75	C
ATOM	467	OE1	GLU	A	75	7.042	11.420	21.066	1.00	87.55	O
ATOM	468	OE2	GLU	A	75	6.072	10.663	22.934	1.00	87.39	O
ATOM	469	C	GLU	A	75	8.436	7.908	19.647	1.00	81.18	C
ATOM	470	O	GLU	A	75	8.049	7.473	18.562	1.00	81.34	O
ATOM	471	N	GLN	A	76	9.249	8.968	19.752	1.00	80.89	N
ATOM	472	CA	GLN	A	76	9.577	9.739	18.545	1.00	81.00	C
ATOM	473	CB	GLN	A	76	10.455	10.976	18.819	1.00	80.64	C
ATOM	474	CG	GLN	A	76	9.682	12.324	18.730	1.00	80.32	C
ATOM	475	CD	GLN	A	76	10.511	13.545	18.240	1.00	80.45	C
ATOM	476	OE1	GLN	A	76	11.267	13.467	17.270	1.00	80.60	O
ATOM	477	NE2	GLN	A	76	10.341	14.673	18.916	1.00	80.12	N
ATOM	478	C	GLN	A	76	10.114	8.827	17.423	1.00	81.41	C
ATOM	479	O	GLN	A	76	10.643	9.297	16.421	1.00	81.26	O
ATOM	480	N	SER	A	77	9.927	7.522	17.613	1.00	82.08	N
ATOM	481	CA	SER	A	77	10.166	6.503	16.608	1.00	83.04	C
ATOM	482	CB	SER	A	77	11.095	5.414	17.158	1.00	83.15	C
ATOM	483	OG	SER	A	77	12.037	4.970	16.191	1.00	82.78	O
ATOM	484	C	SER	A	77	8.826	5.901	16.177	1.00	83.80	C
ATOM	485	O	SER	A	77	8.496	5.897	14.994	1.00	83.79	O
ATOM	486	N	THR	A	78	8.048	5.396	17.132	1.00	84.99	N
ATOM	487	CA	THR	A	78	6.716	4.850	16.819	1.00	86.32	C
ATOM	488	CB	THR	A	78	5.997	4.271	18.089	1.00	86.30	C
ATOM	489	OG1	THR	A	78	5.204	5.283	18.735	1.00	86.91	O
ATOM	490	CG2	THR	A	78	6.992	3.882	19.161	1.00	86.13	C
ATOM	491	C	THR	A	78	5.862	5.924	16.133	1.00	87.20	C
ATOM	492	O	THR	A	78	5.040	5.620	15.256	1.00	87.14	O
ATOM	493	N	LEU	A	79	6.099	7.170	16.561	1.00	88.33	N
ATOM	494	CA	LEU	A	79	5.534	8.399	16.005	1.00	89.50	C
ATOM	495	CB	LEU	A	79	5.436	9.435	17.135	1.00	89.23	C
ATOM	496	CG	LEU	A	79	4.720	10.792	17.014	1.00	89.67	C
ATOM	497	CD1	LEU	A	79	4.391	11.356	18.408	1.00	89.76	C
ATOM	498	CD2	LEU	A	79	5.500	11.834	16.188	1.00	89.02	C
ATOM	499	C	LEU	A	79	6.402	8.959	14.850	1.00	90.55	C
ATOM	500	O	LEU	A	79	6.261	10.129	14.464	1.00	90.30	O
ATOM	501	N	ALA	A	80	7.286	8.123	14.293	1.00	92.01	N

210/396

Figure 3A-10

ATOM	502	CA	ALA	A	80	8.255	8.570	13.277	1.00	93.52	C
ATOM	503	CB	ALA	A	80	9.668	8.571	13.852	1.00	93.59	C
ATOM	504	C	ALA	A	80	8.255	7.779	11.982	1.00	94.50	C
ATOM	505	O	ALA	A	80	8.320	8.367	10.891	1.00	94.76	O
ATOM	506	N	GLN	A	81	8.235	6.450	12.118	1.00	95.54	N
ATOM	507	CA	GLN	A	81	8.289	5.535	10.981	1.00	96.53	C
ATOM	508	CB	GLN	A	81	8.652	4.135	11.438	1.00	96.27	C
ATOM	509	CG	GLN	A	81	7.969	3.731	12.713	1.00	96.47	C
ATOM	510	CD	GLN	A	81	8.721	2.644	13.419	1.00	97.42	C
ATOM	511	OE1	GLN	A	81	9.933	2.539	13.263	1.00	98.13	O
ATOM	512	NE2	GLN	A	81	8.012	1.817	14.190	1.00	98.01	N
ATOM	513	C	GLN	A	81	6.954	5.520	10.261	1.00	97.40	C
ATOM	514	O	GLN	A	81	6.776	4.772	9.293	1.00	97.43	O
ATOM	515	N	MET	A	82	6.021	6.330	10.777	1.00	98.56	N
ATOM	516	CA	MET	A	82	4.840	6.792	10.049	1.00	99.74	C
ATOM	517	CB	MET	A	82	4.211	8.032	10.754	1.00	99.80	C
ATOM	518	CG	MET	A	82	3.033	8.769	10.014	1.00	101.53	C
ATOM	519	SD	MET	A	82	3.348	10.536	9.378	1.00	104.58	S
ATOM	520	CE	MET	A	82	1.627	11.135	8.869	1.00	103.31	C
ATOM	521	C	MET	A	82	5.280	7.086	8.594	1.00	100.15	C
ATOM	522	O	MET	A	82	4.789	6.439	7.651	1.00	100.63	O
ATOM	523	N	TYR	A	83	6.243	8.001	8.428	1.00	100.25	N
ATOM	524	CA	TYR	A	83	6.734	8.421	7.109	1.00	100.35	C
ATOM	525	CB	TYR	A	83	7.954	9.341	7.276	1.00	100.06	C
ATOM	526	CG	TYR	A	83	7.686	10.718	7.886	1.00	98.26	C
ATOM	527	CD1	TYR	A	83	7.191	10.854	9.194	1.00	95.84	C
ATOM	528	CE1	TYR	A	83	6.977	12.102	9.746	1.00	94.37	C
ATOM	529	CZ	TYR	A	83	7.265	13.231	8.996	1.00	94.04	C
ATOM	530	OH	TYR	A	83	7.048	14.472	9.533	1.00	93.82	O
ATOM	531	CE2	TYR	A	83	7.760	13.123	7.711	1.00	94.03	C
ATOM	532	CD2	TYR	A	83	7.975	11.882	7.164	1.00	95.72	C
ATOM	533	C	TYR	A	83	7.114	7.222	6.218	1.00	100.90	C
ATOM	534	O	TYR	A	83	7.668	6.252	6.743	1.00	100.97	O
ATOM	535	N	PRO	A	84	6.819	7.271	4.901	1.00	101.48	N
ATOM	536	CA	PRO	A	84	7.308	6.235	3.966	1.00	101.72	C
ATOM	537	CB	PRO	A	84	6.318	6.305	2.778	1.00	101.81	C
ATOM	538	CG	PRO	A	84	5.676	7.684	2.845	1.00	101.88	C
ATOM	539	CD	PRO	A	84	6.011	8.296	4.201	1.00	101.53	C
ATOM	540	C	PRO	A	84	8.782	6.482	3.544	1.00	101.77	C
ATOM	541	O	PRO	A	84	9.145	7.605	3.175	1.00	101.60	O
ATOM	542	N	LEU	A	85	9.594	5.420	3.611	1.00	101.90	N
ATOM	543	CA	LEU	A	85	11.068	5.488	3.643	1.00	102.04	C
ATOM	544	CB	LEU	A	85	11.664	4.158	4.159	1.00	102.01	C
ATOM	545	CG	LEU	A	85	11.962	2.879	3.342	1.00	101.77	C
ATOM	546	CD1	LEU	A	85	12.178	1.723	4.320	1.00	101.58	C
ATOM	547	CD2	LEU	A	85	10.912	2.488	2.280	1.00	101.23	C
ATOM	548	C	LEU	A	85	11.734	5.908	2.342	1.00	102.23	C
ATOM	549	O	LEU	A	85	12.898	6.333	2.342	1.00	102.11	O
ATOM	550	N	GLN	A	86	11.001	5.744	1.242	1.00	102.47	N
ATOM	551	CA	GLN	A	86	11.352	6.356	-0.036	1.00	102.77	C
ATOM	552	CB	GLN	A	86	11.007	5.428	-1.215	1.00	102.99	C
ATOM	553	CG	GLN	A	86	9.505	5.175	-1.451	1.00	104.48	C
ATOM	554	CD	GLN	A	86	8.984	5.682	-2.820	1.00	106.34	C
ATOM	555	OE1	GLN	A	86	7.838	5.397	-3.184	1.00	106.94	O
ATOM	556	NE2	GLN	A	86	9.817	6.424	-3.564	1.00	106.77	N
ATOM	557	C	GLN	A	86	10.639	7.717	-0.132	1.00	102.48	C

211/396

Figure 3A-11

ATOM	558	O	GLN	A	86	10.239	8.271	0.899	1.00102.71	O
ATOM	559	N	GLU	A	87	10.495	8.252	-1.349	1.00102.00	N
ATOM	560	CA	GLU	A	87	9.764	9.508	-1.602	1.00101.46	C
ATOM	561	CB	GLU	A	87	8.283	9.388	-1.172	1.00101.67	C
ATOM	562	CG	GLU	A	87	7.275	9.967	-2.159	1.00102.16	C
ATOM	563	CD	GLU	A	87	6.516	8.895	-2.914	1.00103.13	C
ATOM	564	OE1	GLU	A	87	6.733	8.746	-4.153	1.00103.54	O
ATOM	565	OE2	GLU	A	87	5.706	8.203	-2.253	1.00103.33	O
ATOM	566	C	GLU	A	87	10.434	10.720	-0.940	1.00100.77	C
ATOM	567	O	GLU	A	87	9.763	11.637	-0.452	1.00100.76	O
ATOM	568	N	ILE	A	88	11.761	10.717	-0.921	1.00 99.85	N
ATOM	569	CA	ILE	A	88	12.506	11.778	-0.262	1.00 98.80	C
ATOM	570	CB	ILE	A	88	12.755	11.455	1.247	1.00 98.72	C
ATOM	571	CG1	ILE	A	88	13.070	9.970	1.471	1.00 98.46	C
ATOM	572	CD1	ILE	A	88	12.608	9.427	2.837	1.00 97.59	C
ATOM	573	CG2	ILE	A	88	11.545	11.850	2.079	1.00 98.50	C
ATOM	574	C	ILE	A	88	13.796	12.078	-1.012	1.00 98.19	C
ATOM	575	O	ILE	A	88	14.619	11.184	-1.255	1.00 98.19	O
ATOM	576	N	GLN	A	89	13.937	13.341	-1.407	1.00 97.15	N
ATOM	577	CA	GLN	A	89	15.169	13.835	-2.025	1.00 96.20	C
ATOM	578	CB	GLN	A	89	14.867	14.884	-3.142	1.00 96.46	C
ATOM	579	CG	GLN	A	89	13.620	14.551	-4.061	1.00 96.12	C
ATOM	580	CD	GLN	A	89	13.846	14.697	-5.600	1.00 95.63	C
ATOM	581	OE1	GLN	A	89	13.972	13.695	-6.324	1.00 94.05	O
ATOM	582	NE2	GLN	A	89	13.844	15.935	-6.087	1.00 95.28	N
ATOM	583	C	GLN	A	89	16.166	14.296	-0.909	1.00 95.33	C
ATOM	584	O	GLN	A	89	16.379	13.537	0.039	1.00 95.14	O
ATOM	585	N	ASN	A	90	16.734	15.509	-0.994	1.00 94.24	N
ATOM	586	CA	ASN	A	90	17.864	15.966	-0.128	1.00 93.16	C
ATOM	587	CB	ASN	A	90	17.658	17.413	0.403	1.00 93.19	C
ATOM	588	CG	ASN	A	90	18.990	18.203	0.573	1.00 91.93	C
ATOM	589	OD1	ASN	A	90	19.278	19.150	-0.170	1.00 89.63	O
ATOM	590	ND2	ASN	A	90	19.771	17.829	1.575	1.00 90.43	N
ATOM	591	C	ASN	A	90	18.368	15.005	0.978	1.00 92.50	C
ATOM	592	O	ASN	A	90	18.246	15.273	2.180	1.00 92.05	O
ATOM	593	N	LEU	A	91	18.930	13.889	0.496	1.00 91.76	N
ATOM	594	CA	LEU	A	91	19.635	12.829	1.238	1.00 90.85	C
ATOM	595	CB	LEU	A	91	21.104	12.713	0.772	1.00 90.99	C
ATOM	596	CG	LEU	A	91	21.997	13.846	0.183	1.00 91.58	C
ATOM	597	CD1	LEU	A	91	21.877	14.010	-1.360	1.00 90.89	C
ATOM	598	CD2	LEU	A	91	21.897	15.222	0.900	1.00 91.64	C
ATOM	599	C	LEU	A	91	19.564	12.865	2.759	1.00 90.20	C
ATOM	600	O	LEU	A	91	18.855	12.076	3.379	1.00 90.16	O
ATOM	601	N	THR	A	92	20.312	13.782	3.354	1.00 89.42	N
ATOM	602	CA	THR	A	92	20.329	13.975	4.805	1.00 88.75	C
ATOM	603	CB	THR	A	92	20.988	15.351	5.113	1.00 88.91	C
ATOM	604	OG1	THR	A	92	22.417	15.220	5.008	1.00 89.06	O
ATOM	605	CG2	THR	A	92	20.737	15.828	6.558	1.00 88.52	C
ATOM	606	C	THR	A	92	18.937	13.812	5.461	1.00 88.02	C
ATOM	607	O	THR	A	92	18.819	13.338	6.601	1.00 87.96	O
ATOM	608	N	VAL	A	93	17.896	14.177	4.713	1.00 86.85	N
ATOM	609	CA	VAL	A	93	16.517	14.080	5.193	1.00 85.45	C
ATOM	610	CB	VAL	A	93	15.525	14.871	4.284	1.00 85.56	C
ATOM	611	CG1	VAL	A	93	15.932	16.343	4.215	1.00 85.20	C
ATOM	612	CG2	VAL	A	93	15.434	14.260	2.884	1.00 85.23	C
ATOM	613	C	VAL	A	93	16.066	12.628	5.431	1.00 84.32	C

212/396

Figure 3A-12

ATOM	614	O	VAL	A	93	15.377	12.354	6.426	1.00	84.32	O
ATOM	615	N	LYS	A	94	16.469	11.716	4.538	1.00	82.48	N
ATOM	616	CA	LYS	A	94	16.199	10.280	4.692	1.00	80.82	C
ATOM	617	CB	LYS	A	94	16.278	9.534	3.339	1.00	80.82	C
ATOM	618	CG	LYS	A	94	17.323	8.383	3.214	1.00	79.44	C
ATOM	619	CD	LYS	A	94	17.654	8.055	1.744	1.00	77.23	C
ATOM	620	CE	LYS	A	94	18.833	7.086	1.603	1.00	75.92	C
ATOM	621	NZ	LYS	A	94	18.898	6.411	0.262	1.00	73.66	N
ATOM	622	C	LYS	A	94	17.142	9.658	5.703	1.00	79.95	C
ATOM	623	O	LYS	A	94	16.746	8.779	6.462	1.00	79.36	O
ATOM	624	N	LEU	A	95	18.388	10.125	5.705	1.00	78.96	N
ATOM	625	CA	LEU	A	95	19.423	9.498	6.514	1.00	78.25	C
ATOM	626	CB	LEU	A	95	20.792	9.564	5.821	1.00	78.34	C
ATOM	627	CG	LEU	A	95	21.709	10.759	6.043	1.00	79.02	C
ATOM	628	CD1	LEU	A	95	22.758	10.459	7.115	1.00	79.87	C
ATOM	629	CD2	LEU	A	95	22.376	11.124	4.736	1.00	80.31	C
ATOM	630	C	LEU	A	95	19.447	10.027	7.953	1.00	77.51	C
ATOM	631	O	LEU	A	95	20.085	9.421	8.849	1.00	77.37	O
ATOM	632	N	GLN	A	96	18.756	11.156	8.158	1.00	76.31	N
ATOM	633	CA	GLN	A	96	18.421	11.628	9.496	1.00	75.17	C
ATOM	634	CB	GLN	A	96	18.159	13.132	9.504	1.00	74.84	C
ATOM	635	CG	GLN	A	96	19.401	13.961	9.765	1.00	74.17	C
ATOM	636	CD	GLN	A	96	19.099	15.421	10.044	1.00	74.27	C
ATOM	637	OE1	GLN	A	96	19.194	16.269	9.153	1.00	73.65	O
ATOM	638	NE2	GLN	A	96	18.742	15.723	11.287	1.00	74.73	N
ATOM	639	C	GLN	A	96	17.197	10.828	9.929	1.00	74.73	C
ATOM	640	O	GLN	A	96	17.024	10.491	11.111	1.00	74.40	O
ATOM	641	N	LEU	A	97	16.369	10.487	8.944	1.00	74.13	N
ATOM	642	CA	LEU	A	97	15.241	9.607	9.183	1.00	73.82	C
ATOM	643	CB	LEU	A	97	14.333	9.533	7.956	1.00	73.57	C
ATOM	644	CG	LEU	A	97	12.878	10.024	8.048	1.00	73.36	C
ATOM	645	CD1	LEU	A	97	12.067	9.424	9.236	1.00	73.61	C
ATOM	646	CD2	LEU	A	97	12.847	11.546	8.072	1.00	72.20	C
ATOM	647	C	LEU	A	97	15.773	8.241	9.500	1.00	73.76	C
ATOM	648	O	LEU	A	97	15.197	7.525	10.299	1.00	73.30	O
ATOM	649	N	GLN	A	98	16.898	7.915	8.865	1.00	74.24	N
ATOM	650	CA	GLN	A	98	17.491	6.581	8.886	1.00	74.59	C
ATOM	651	CB	GLN	A	98	18.766	6.522	8.025	1.00	74.59	C
ATOM	652	CG	GLN	A	98	18.781	5.478	6.883	1.00	74.11	C
ATOM	653	CD	GLN	A	98	19.758	5.850	5.747	1.00	73.87	C
ATOM	654	OE1	GLN	A	98	20.845	6.361	6.007	1.00	74.72	O
ATOM	655	NE2	GLN	A	98	19.368	5.590	4.500	1.00	72.93	N
ATOM	656	C	GLN	A	98	17.794	6.149	10.297	1.00	74.84	C
ATOM	657	O	GLN	A	98	17.232	5.170	10.772	1.00	74.71	O
ATOM	658	N	ALA	A	99	18.668	6.876	10.978	1.00	75.55	N
ATOM	659	CA	ALA	A	99	19.027	6.471	12.332	1.00	76.86	C
ATOM	660	CB	ALA	A	99	20.164	7.323	12.893	1.00	77.26	C
ATOM	661	C	ALA	A	99	17.809	6.550	13.238	1.00	77.52	C
ATOM	662	O	ALA	A	99	17.745	5.851	14.264	1.00	77.51	O
ATOM	663	N	LEU	A	100	16.849	7.392	12.822	1.00	78.22	N
ATOM	664	CA	LEU	A	100	15.634	7.706	13.587	1.00	78.39	C
ATOM	665	CB	LEU	A	100	15.052	9.060	13.151	1.00	78.01	C
ATOM	666	CG	LEU	A	100	14.987	10.083	14.293	1.00	78.43	C
ATOM	667	CD1	LEU	A	100	14.264	11.374	13.893	1.00	78.36	C
ATOM	668	CD2	LEU	A	100	14.370	9.491	15.574	1.00	78.13	C
ATOM	669	C	LEU	A	100	14.548	6.611	13.586	1.00	78.71	C

213/396

Figure 3A-13

ATOM	670	O	LEU	A	100	14.004	6.279	14.652	1.00	78.90	O
ATOM	671	N	GLN	A	101	14.245	6.053	12.404	1.00	78.97	N
ATOM	672	CA	GLN	A	101	13.218	5.011	12.243	1.00	78.85	C
ATOM	673	CB	GLN	A	101	13.133	4.546	10.798	1.00	78.92	C
ATOM	674	CG	GLN	A	101	12.036	5.188	9.992	1.00	80.43	C
ATOM	675	CD	GLN	A	101	12.500	5.498	8.586	1.00	82.49	C
ATOM	676	OE1	GLN	A	101	12.233	4.736	7.638	1.00	82.97	O
ATOM	677	NE2	GLN	A	101	13.224	6.601	8.444	1.00	82.85	N
ATOM	678	C	GLN	A	101	13.562	3.815	13.076	1.00	78.62	C
ATOM	679	O	GLN	A	101	12.705	3.004	13.389	1.00	78.81	O
ATOM	680	N	GLN	A	102	14.836	3.719	13.427	1.00	78.38	N
ATOM	681	CA	GLN	A	102	15.375	2.534	14.048	1.00	78.10	C
ATOM	682	CB	GLN	A	102	16.884	2.462	13.797	1.00	78.30	C
ATOM	683	CG	GLN	A	102	17.236	2.208	12.303	1.00	78.71	C
ATOM	684	CD	GLN	A	102	18.493	1.346	12.116	1.00	79.03	C
ATOM	685	OE1	GLN	A	102	19.318	1.268	13.032	1.00	79.33	O
ATOM	686	NE2	GLN	A	102	18.639	0.703	10.937	1.00	77.56	N
ATOM	687	C	GLN	A	102	15.009	2.482	15.521	1.00	77.65	C
ATOM	688	O	GLN	A	102	15.620	3.151	16.352	1.00	77.15	O
ATOM	689	N	ASN	A	103	13.960	1.709	15.807	1.00	77.66	N
ATOM	690	CA	ASN	A	103	13.509	1.443	17.174	1.00	77.64	C
ATOM	691	CB	ASN	A	103	12.124	0.749	17.231	1.00	77.70	C
ATOM	692	CG	ASN	A	103	11.956	-0.371	16.191	1.00	77.85	C
ATOM	693	OD1	ASN	A	103	11.226	-0.210	15.207	1.00	77.10	O
ATOM	694	ND2	ASN	A	103	12.606	-1.519	16.426	1.00	77.78	N
ATOM	695	C	ASN	A	103	14.574	0.625	17.873	1.00	77.34	C
ATOM	696	O	ASN	A	103	14.827	-0.525	17.504	1.00	77.48	O
ATOM	697	N	GLY	A	104	15.211	1.237	18.865	1.00	76.90	N
ATOM	698	CA	GLY	A	104	16.450	0.710	19.394	1.00	76.29	C
ATOM	699	C	GLY	A	104	16.270	-0.449	20.346	1.00	75.86	C
ATOM	700	O	GLY	A	104	15.499	-1.381	20.088	1.00	75.69	O
ATOM	701	N	SER	A	105	17.021	-0.382	21.446	1.00	75.54	N
ATOM	702	CA	SER	A	105	16.912	-1.314	22.563	1.00	74.67	C
ATOM	703	CB	SER	A	105	18.176	-1.275	23.430	1.00	74.81	C
ATOM	704	OG	SER	A	105	18.699	-2.574	23.658	1.00	73.50	O
ATOM	705	C	SER	A	105	15.676	-0.916	23.356	1.00	74.19	C
ATOM	706	O	SER	A	105	15.763	-0.267	24.400	1.00	74.19	O
ATOM	707	N	SER	A	106	14.533	-1.301	22.790	1.00	73.52	N
ATOM	708	CA	SER	A	106	13.186	-1.061	23.300	1.00	72.65	C
ATOM	709	CB	SER	A	106	12.583	0.189	22.640	1.00	72.67	C
ATOM	710	OG	SER	A	106	13.086	0.387	21.320	1.00	72.99	O
ATOM	711	C	SER	A	106	12.408	-2.321	22.906	1.00	71.79	C
ATOM	712	O	SER	A	106	11.336	-2.634	23.438	1.00	71.66	O
ATOM	713	N	VAL	A	107	12.999	-3.041	21.961	1.00	70.47	N
ATOM	714	CA	VAL	A	107	12.541	-4.330	21.523	1.00	69.54	C
ATOM	715	CB	VAL	A	107	13.568	-4.919	20.576	1.00	69.57	C
ATOM	716	CG1	VAL	A	107	13.318	-6.413	20.333	1.00	69.44	C
ATOM	717	CG2	VAL	A	107	13.577	-4.128	19.279	1.00	70.21	C
ATOM	718	C	VAL	A	107	12.425	-5.244	22.698	1.00	69.05	C
ATOM	719	O	VAL	A	107	12.298	-6.445	22.537	1.00	68.91	O
ATOM	720	N	LEU	A	108	12.475	-4.678	23.890	1.00	69.07	N
ATOM	721	CA	LEU	A	108	12.523	-5.493	25.089	1.00	69.52	C
ATOM	722	CB	LEU	A	108	13.886	-5.379	25.801	1.00	69.73	C
ATOM	723	CG	LEU	A	108	15.206	-5.520	25.039	1.00	69.14	C
ATOM	724	CD1	LEU	A	108	15.758	-4.118	24.882	1.00	68.92	C
ATOM	725	CD2	LEU	A	108	16.211	-6.475	25.717	1.00	67.13	C

214/396

Figure 3A-14

ATOM	726	C	LEU	A	108	11.426	-5.170	26.072	1.00	69.71	C
ATOM	727	O	LEU	A	108	10.941	-4.038	26.137	1.00	69.39	O
ATOM	728	N	SER	A	109	11.066	-6.201	26.835	1.00	70.38	N
ATOM	729	CA	SER	A	109	10.161	-6.113	27.976	1.00	71.42	C
ATOM	730	CB	SER	A	109	10.043	-7.506	28.650	1.00	71.06	C
ATOM	731	OG	SER	A	109	9.298	-7.504	29.857	1.00	70.25	O
ATOM	732	C	SER	A	109	10.764	-5.079	28.919	1.00	72.32	C
ATOM	733	O	SER	A	109	11.811	-5.342	29.486	1.00	72.81	O
ATOM	734	N	GLU	A	110	10.161	-3.894	29.051	1.00	73.19	N
ATOM	735	CA	GLU	A	110	10.701	-2.916	29.987	1.00	74.21	C
ATOM	736	CB	GLU	A	110	9.698	-1.809	30.345	1.00	74.83	C
ATOM	737	CG	GLU	A	110	9.972	-1.078	31.679	1.00	77.54	C
ATOM	738	CD	GLU	A	110	10.780	0.238	31.562	1.00	80.27	C
ATOM	739	OE1	GLU	A	110	11.185	0.629	30.426	1.00	80.06	O
ATOM	740	OE2	GLU	A	110	11.012	0.887	32.630	1.00	80.50	O
ATOM	741	C	GLU	A	110	11.073	-3.733	31.197	1.00	74.24	C
ATOM	742	O	GLU	A	110	12.224	-3.720	31.628	1.00	74.03	O
ATOM	743	N	ASP	A	111	10.106	-4.498	31.696	1.00	74.69	N
ATOM	744	CA	ASP	A	111	10.338	-5.445	32.794	1.00	75.33	C
ATOM	745	CB	ASP	A	111	9.215	-6.489	32.824	1.00	75.92	C
ATOM	746	CG	ASP	A	111	7.882	-5.908	33.288	1.00	78.10	C
ATOM	747	OD1	ASP	A	111	7.767	-4.644	33.386	1.00	79.35	O
ATOM	748	OD2	ASP	A	111	6.904	-6.658	33.580	1.00	80.20	O
ATOM	749	C	ASP	A	111	11.705	-6.147	32.740	1.00	74.67	C
ATOM	750	O	ASP	A	111	12.137	-6.744	33.733	1.00	74.35	O
ATOM	751	N	LYS	A	112	12.357	-6.041	31.578	1.00	74.11	N
ATOM	752	CA	LYS	A	112	13.614	-6.715	31.251	1.00	73.85	C
ATOM	753	CB	LYS	A	112	13.362	-7.933	30.319	1.00	73.68	C
ATOM	754	CG	LYS	A	112	14.180	-8.011	29.041	1.00	73.67	C
ATOM	755	CD	LYS	A	112	13.283	-8.113	27.811	1.00	75.03	C
ATOM	756	CE	LYS	A	112	12.926	-9.585	27.415	1.00	77.01	C
ATOM	757	NZ	LYS	A	112	13.038	-9.930	25.925	1.00	75.90	N
ATOM	758	C	LYS	A	112	14.709	-5.735	30.736	1.00	73.60	C
ATOM	759	O	LYS	A	112	15.835	-5.745	31.257	1.00	73.87	O
ATOM	760	N	SER	A	113	14.404	-4.882	29.751	1.00	72.91	N
ATOM	761	CA	SER	A	113	15.378	-3.851	29.339	1.00	72.07	C
ATOM	762	CB	SER	A	113	14.814	-2.879	28.286	1.00	72.10	C
ATOM	763	OG	SER	A	113	13.512	-2.403	28.594	1.00	72.23	O
ATOM	764	C	SER	A	113	15.927	-3.112	30.579	1.00	71.52	C
ATOM	765	O	SER	A	113	17.108	-2.725	30.610	1.00	71.56	O
ATOM	766	N	LYS	A	114	15.054	-2.951	31.590	1.00	70.50	N
ATOM	767	CA	LYS	A	114	15.425	-2.589	32.958	1.00	68.87	C
ATOM	768	CB	LYS	A	114	14.311	-2.946	33.955	1.00	68.92	C
ATOM	769	CG	LYS	A	114	13.445	-1.756	34.456	1.00	69.11	C
ATOM	770	CD	LYS	A	114	12.789	-1.960	35.848	1.00	67.92	C
ATOM	771	CE	LYS	A	114	12.711	-3.435	36.276	1.00	68.16	C
ATOM	772	NZ	LYS	A	114	13.982	-4.019	36.850	1.00	67.04	N
ATOM	773	C	LYS	A	114	16.604	-3.447	33.246	1.00	67.79	C
ATOM	774	O	LYS	A	114	17.725	-3.025	33.009	1.00	67.86	O
ATOM	775	N	ARG	A	115	16.333	-4.681	33.674	1.00	66.63	N
ATOM	776	CA	ARG	A	115	17.350	-5.640	34.131	1.00	65.74	C
ATOM	777	CB	ARG	A	115	16.880	-7.090	33.933	1.00	66.04	C
ATOM	778	CG	ARG	A	115	17.908	-8.160	34.257	1.00	68.21	C
ATOM	779	CD	ARG	A	115	17.846	-8.688	35.690	1.00	73.38	C
ATOM	780	NE	ARG	A	115	19.065	-9.412	36.082	1.00	76.30	N
ATOM	781	CZ	ARG	A	115	20.194	-8.837	36.534	1.00	77.10	C

215/396

Figure 3A-15

ATOM	782	NH1	ARG	A	115	21.239	-9.595	36.866	1.00	76.46	N
ATOM	783	NH2	ARG	A	115	20.284	-7.511	36.657	1.00	77.21	N
ATOM	784	C	ARG	A	115	18.703	-5.407	33.483	1.00	64.47	C
ATOM	785	O	ARG	A	115	19.702	-5.354	34.188	1.00	64.39	O
ATOM	786	N	LEU	A	116	18.721	-5.235	32.156	1.00	63.12	N
ATOM	787	CA	LEU	A	116	19.951	-4.933	31.411	1.00	61.53	C
ATOM	788	CB	LEU	A	116	19.699	-4.804	29.907	1.00	61.67	C
ATOM	789	CG	LEU	A	116	20.979	-4.550	29.106	1.00	61.43	C
ATOM	790	CD1	LEU	A	116	21.723	-5.859	28.769	1.00	62.00	C
ATOM	791	CD2	LEU	A	116	20.692	-3.735	27.860	1.00	61.86	C
ATOM	792	C	LEU	A	116	20.626	-3.676	31.927	1.00	60.35	C
ATOM	793	O	LEU	A	116	21.660	-3.753	32.600	1.00	60.41	O
ATOM	794	N	ASN	A	117	20.045	-2.522	31.621	1.00	58.34	N
ATOM	795	CA	ASN	A	117	20.559	-1.274	32.158	1.00	56.85	C
ATOM	796	CB	ASN	A	117	19.456	-0.248	32.226	1.00	57.05	C
ATOM	797	CG	ASN	A	117	18.930	0.083	30.863	1.00	59.49	C
ATOM	798	OD1	ASN	A	117	18.554	1.223	30.588	1.00	62.91	O
ATOM	799	ND2	ASN	A	117	18.923	-0.912	29.971	1.00	61.46	N
ATOM	800	C	ASN	A	117	21.192	-1.467	33.512	1.00	55.08	C
ATOM	801	O	ASN	A	117	22.261	-0.966	33.779	1.00	55.16	O
ATOM	802	N	THR	A	118	20.560	-2.263	34.343	1.00	53.04	N
ATOM	803	CA	THR	A	118	21.020	-2.405	35.688	1.00	51.84	C
ATOM	804	CB	THR	A	118	19.772	-2.454	36.652	1.00	51.94	C
ATOM	805	OG1	THR	A	118	19.851	-1.393	37.638	1.00	50.93	O
ATOM	806	CG2	THR	A	118	19.601	-3.817	37.412	1.00	51.32	C
ATOM	807	C	THR	A	118	22.107	-3.513	35.824	1.00	51.65	C
ATOM	808	O	THR	A	118	22.703	-3.720	36.907	1.00	51.45	O
ATOM	809	N	ILE	A	119	22.400	-4.196	34.715	1.00	50.85	N
ATOM	810	CA	ILE	A	119	23.617	-5.002	34.642	1.00	50.11	C
ATOM	811	CB	ILE	A	119	23.556	-6.093	33.564	1.00	50.09	C
ATOM	812	CG1	ILE	A	119	22.397	-7.030	33.801	1.00	50.34	C
ATOM	813	CD1	ILE	A	119	21.727	-7.382	32.526	1.00	51.65	C
ATOM	814	CG2	ILE	A	119	24.822	-6.922	33.561	1.00	50.15	C
ATOM	815	C	ILE	A	119	24.663	-3.990	34.254	1.00	49.64	C
ATOM	816	O	ILE	A	119	25.571	-3.666	35.032	1.00	49.46	O
ATOM	817	N	LEU	A	120	24.518	-3.463	33.049	1.00	48.78	N
ATOM	818	CA	LEU	A	120	25.432	-2.445	32.617	1.00	48.53	C
ATOM	819	CB	LEU	A	120	24.759	-1.539	31.621	1.00	48.29	C
ATOM	820	CG	LEU	A	120	24.472	-2.293	30.356	1.00	48.15	C
ATOM	821	CD1	LEU	A	120	23.215	-1.699	29.789	1.00	49.59	C
ATOM	822	CD2	LEU	A	120	25.644	-2.185	29.392	1.00	47.39	C
ATOM	823	C	LEU	A	120	25.874	-1.644	33.834	1.00	48.59	C
ATOM	824	O	LEU	A	120	27.070	-1.533	34.087	1.00	48.83	O
ATOM	825	N	ASN	A	121	24.905	-1.119	34.588	1.00	48.27	N
ATOM	826	CA	ASN	A	121	25.185	-0.309	35.746	1.00	48.19	C
ATOM	827	CB	ASN	A	121	23.936	-0.070	36.568	1.00	48.67	C
ATOM	828	CG	ASN	A	121	23.331	1.277	36.311	1.00	50.87	C
ATOM	829	OD1	ASN	A	121	23.823	2.018	35.469	1.00	54.69	O
ATOM	830	ND2	ASN	A	121	22.237	1.607	37.018	1.00	53.06	N
ATOM	831	C	ASN	A	121	26.183	-1.016	36.604	1.00	48.07	C
ATOM	832	O	ASN	A	121	27.314	-0.519	36.748	1.00	49.04	O
ATOM	833	N	THR	A	122	25.780	-2.169	37.159	1.00	46.63	N
ATOM	834	CA	THR	A	122	26.611	-2.905	38.116	1.00	45.56	C
ATOM	835	CB	THR	A	122	26.085	-4.336	38.345	1.00	46.03	C
ATOM	836	OG1	THR	A	122	24.742	-4.295	38.864	1.00	47.64	O
ATOM	837	CG2	THR	A	122	26.945	-5.115	39.397	1.00	44.16	C

216/396

Figure 3A-16

ATOM	838	C	THR	A	122	27.916	-3.058	37.454	1.00	44.58	C
ATOM	839	O	THR	A	122	28.927	-2.511	37.878	1.00	44.67	O
ATOM	840	N	MET	A	123	27.839	-3.811	36.371	1.00	43.34	N
ATOM	841	CA	MET	A	123	28.960	-4.206	35.575	1.00	42.31	C
ATOM	842	CB	MET	A	123	28.429	-4.602	34.227	1.00	42.15	C
ATOM	843	CG	MET	A	123	28.481	-6.054	33.970	1.00	42.05	C
ATOM	844	SD	MET	A	123	29.224	-6.145	32.351	1.00	44.31	S
ATOM	845	CE	MET	A	123	28.216	-4.940	31.413	1.00	43.46	C
ATOM	846	C	MET	A	123	29.985	-3.097	35.452	1.00	41.63	C
ATOM	847	O	MET	A	123	31.178	-3.371	35.428	1.00	41.06	O
ATOM	848	N	SER	A	124	29.503	-1.853	35.388	1.00	41.17	N
ATOM	849	CA	SER	A	124	30.359	-0.680	35.399	1.00	40.97	C
ATOM	850	CB	SER	A	124	29.584	0.606	35.139	1.00	40.95	C
ATOM	851	OG	SER	A	124	30.445	1.730	35.288	1.00	40.04	O
ATOM	852	C	SER	A	124	30.917	-0.577	36.772	1.00	41.07	C
ATOM	853	O	SER	A	124	31.921	-1.217	37.079	1.00	41.16	O
ATOM	854	N	THR	A	125	30.245	0.228	37.597	1.00	41.00	N
ATOM	855	CA	THR	A	125	30.659	0.442	38.983	1.00	41.08	C
ATOM	856	CB	THR	A	125	29.441	0.457	39.957	1.00	41.40	C
ATOM	857	OG1	THR	A	125	29.189	-0.868	40.460	1.00	41.26	O
ATOM	858	CG2	THR	A	125	28.158	0.812	39.192	1.00	41.84	C
ATOM	859	C	THR	A	125	31.638	-0.652	39.354	1.00	40.36	C
ATOM	860	O	THR	A	125	32.839	-0.416	39.350	1.00	40.80	O
ATOM	861	N	ILE	A	126	31.110	-1.844	39.617	1.00	39.20	N
ATOM	862	CA	ILE	A	126	31.898	-3.035	39.845	1.00	38.73	C
ATOM	863	CB	ILE	A	126	31.209	-4.234	39.148	1.00	39.02	C
ATOM	864	CG1	ILE	A	126	31.085	-5.423	40.112	1.00	40.06	C
ATOM	865	CD1	ILE	A	126	32.376	-6.174	40.368	1.00	40.92	C
ATOM	866	CG2	ILE	A	126	31.852	-4.596	37.818	1.00	39.31	C
ATOM	867	C	ILE	A	126	33.402	-2.868	39.526	1.00	38.09	C
ATOM	868	O	ILE	A	126	34.184	-2.640	40.434	1.00	38.54	O
ATOM	869	N	TYR	A	127	33.795	-2.923	38.260	1.00	37.08	N
ATOM	870	CA	TYR	A	127	35.138	-2.542	37.822	1.00	36.26	C
ATOM	871	CB	TYR	A	127	35.107	-2.429	36.305	1.00	36.26	C
ATOM	872	CG	TYR	A	127	36.311	-1.831	35.606	1.00	36.13	C
ATOM	873	CD1	TYR	A	127	36.520	-0.460	35.565	1.00	35.80	C
ATOM	874	CE1	TYR	A	127	37.614	0.074	34.890	1.00	34.28	C
ATOM	875	CZ	TYR	A	127	38.478	-0.749	34.210	1.00	31.92	C
ATOM	876	OH	TYR	A	127	39.556	-0.215	33.557	1.00	29.70	O
ATOM	877	CE2	TYR	A	127	38.279	-2.093	34.212	1.00	33.37	C
ATOM	878	CD2	TYR	A	127	37.195	-2.636	34.906	1.00	35.49	C
ATOM	879	C	TYR	A	127	35.632	-1.239	38.459	1.00	35.97	C
ATOM	880	O	TYR	A	127	36.524	-1.243	39.259	1.00	35.19	O
ATOM	881	N	SER	A	128	35.025	-0.120	38.136	1.00	36.58	N
ATOM	882	CA	SER	A	128	35.496	1.127	38.683	1.00	37.80	C
ATOM	883	CB	SER	A	128	34.805	2.303	37.999	1.00	38.14	C
ATOM	884	OG	SER	A	128	35.758	3.295	37.605	1.00	39.66	O
ATOM	885	C	SER	A	128	35.272	1.222	40.173	1.00	38.33	C
ATOM	886	O	SER	A	128	35.039	2.302	40.695	1.00	38.42	O
ATOM	887	N	THR	A	129	35.346	0.110	40.880	1.00	39.41	N
ATOM	888	CA	THR	A	129	35.035	0.158	42.306	1.00	41.11	C
ATOM	889	CB	THR	A	129	33.490	0.036	42.509	1.00	40.99	C
ATOM	890	OG1	THR	A	129	32.981	1.147	43.266	1.00	40.58	O
ATOM	891	CG2	THR	A	129	33.158	-1.136	43.364	1.00	41.08	C
ATOM	892	C	THR	A	129	35.795	-0.923	43.082	1.00	42.36	C
ATOM	893	O	THR	A	129	36.167	-0.744	44.262	1.00	42.42	O

217/396

Figure 3A-17

ATOM	894	N	GLY	A	130	36.017	-2.036	42.392	1.00	43.78	N
ATOM	895	CA	GLY	A	130	36.649	-3.212	42.947	1.00	45.72	C
ATOM	896	C	GLY	A	130	38.022	-2.857	43.383	1.00	47.36	C
ATOM	897	O	GLY	A	130	38.804	-2.265	42.655	1.00	47.55	O
ATOM	898	N	LYS	A	131	38.290	-3.163	44.630	1.00	49.51	N
ATOM	899	CA	LYS	A	131	39.633	-3.012	45.161	1.00	51.56	C
ATOM	900	CB	LYS	A	131	39.570	-2.443	46.607	1.00	51.75	C
ATOM	901	CG	LYS	A	131	38.453	-1.375	46.872	1.00	52.52	C
ATOM	902	CD	LYS	A	131	38.944	-0.175	47.750	1.00	54.66	C
ATOM	903	CE	LYS	A	131	37.791	0.822	48.145	1.00	55.19	C
ATOM	904	NZ	LYS	A	131	38.093	1.821	49.245	1.00	54.22	N
ATOM	905	C	LYS	A	131	40.132	-4.456	45.124	1.00	52.32	C
ATOM	906	O	LYS	A	131	39.322	-5.355	44.879	1.00	53.27	O
ATOM	907	N	VAL	A	132	41.416	-4.713	45.325	1.00	52.87	N
ATOM	908	CA	VAL	A	132	41.782	-6.041	45.829	1.00	54.19	C
ATOM	909	CB	VAL	A	132	42.713	-6.812	44.885	1.00	54.12	C
ATOM	910	CG1	VAL	A	132	41.961	-7.285	43.662	1.00	53.88	C
ATOM	911	CG2	VAL	A	132	43.897	-5.954	44.488	1.00	54.90	C
ATOM	912	C	VAL	A	132	42.425	-5.855	47.205	1.00	55.08	C
ATOM	913	O	VAL	A	132	42.960	-4.777	47.471	1.00	55.61	O
ATOM	914	N	CYS	A	133	42.375	-6.862	48.086	1.00	55.74	N
ATOM	915	CA	CYS	A	133	43.041	-6.723	49.392	1.00	56.39	C
ATOM	916	CB	CYS	A	133	42.073	-6.888	50.574	1.00	56.49	C
ATOM	917	SG	CYS	A	133	41.981	-5.324	51.535	1.00	60.72	S
ATOM	918	C	CYS	A	133	44.331	-7.520	49.588	1.00	56.01	C
ATOM	919	O	CYS	A	133	44.368	-8.722	49.337	1.00	56.09	O
ATOM	920	N	ASN	A	134	45.368	-6.816	50.052	1.00	55.87	N
ATOM	921	CA	ASN	A	134	46.724	-7.337	50.273	1.00	55.98	C
ATOM	922	CB	ASN	A	134	47.578	-6.228	50.895	1.00	56.18	C
ATOM	923	CG	ASN	A	134	48.981	-6.686	51.261	1.00	56.69	C
ATOM	924	OD1	ASN	A	134	49.279	-7.892	51.303	1.00	55.20	O
ATOM	925	ND2	ASN	A	134	49.857	-5.710	51.544	1.00	57.45	N
ATOM	926	C	ASN	A	134	46.762	-8.576	51.162	1.00	55.89	C
ATOM	927	O	ASN	A	134	46.405	-8.490	52.327	1.00	56.16	O
ATOM	928	N	PRO	A	135	47.243	-9.713	50.654	1.00	55.82	N
ATOM	929	CA	PRO	A	135	46.921	-11.004	51.280	1.00	55.68	C
ATOM	930	CB	PRO	A	135	47.569	-12.053	50.343	1.00	55.71	C
ATOM	931	CG	PRO	A	135	47.920	-11.326	49.119	1.00	55.81	C
ATOM	932	CD	PRO	A	135	48.165	-9.879	49.517	1.00	55.82	C
ATOM	933	C	PRO	A	135	47.499	-11.090	52.683	1.00	55.32	C
ATOM	934	O	PRO	A	135	46.872	-11.694	53.562	1.00	55.39	O
ATOM	935	N	ASP	A	136	48.663	-10.475	52.878	1.00	54.50	N
ATOM	936	CA	ASP	A	136	49.297	-10.460	54.171	1.00	53.90	C
ATOM	937	CB	ASP	A	136	50.773	-10.110	54.018	1.00	54.93	C
ATOM	938	CG	ASP	A	136	51.023	-8.600	53.963	1.00	56.90	C
ATOM	939	OD1	ASP	A	136	51.443	-8.087	52.889	1.00	60.22	O
ATOM	940	OD2	ASP	A	136	50.851	-7.855	54.955	1.00	57.35	O
ATOM	941	C	ASP	A	136	48.589	-9.499	55.115	1.00	52.68	C
ATOM	942	O	ASP	A	136	48.452	-9.815	56.300	1.00	51.99	O
ATOM	943	N	ASN	A	137	48.134	-8.357	54.560	1.00	51.82	N
ATOM	944	CA	ASN	A	137	47.447	-7.237	55.269	1.00	50.98	C
ATOM	945	CB	ASN	A	137	48.325	-5.968	55.250	1.00	50.45	C
ATOM	946	CG	ASN	A	137	47.748	-4.815	56.065	1.00	48.06	C
ATOM	947	OD1	ASN	A	137	48.348	-3.745	56.143	1.00	45.25	O
ATOM	948	ND2	ASN	A	137	46.597	-5.029	56.670	1.00	45.20	N
ATOM	949	C	ASN	A	137	46.050	-6.866	54.728	1.00	51.01	C

218/396

Figure 3A-18

ATOM	950	O	ASN	A	137	45.937	-5.967	53.888	1.00	51.35	O
ATOM	951	N	PRO	A	138	45.000	-7.550	55.185	1.00	50.85	N
ATOM	952	CA	PRO	A	138	43.616	-7.197	54.876	1.00	51.06	C
ATOM	953	CB	PRO	A	138	42.875	-7.821	56.039	1.00	50.91	C
ATOM	954	CG	PRO	A	138	43.604	-9.083	56.267	1.00	51.04	C
ATOM	955	CD	PRO	A	138	45.043	-8.776	55.991	1.00	51.13	C
ATOM	956	C	PRO	A	138	43.295	-5.708	54.839	1.00	51.42	C
ATOM	957	O	PRO	A	138	42.230	-5.334	54.324	1.00	51.25	O
ATOM	958	N	GLN	A	139	44.181	-4.878	55.390	1.00	51.73	N
ATOM	959	CA	GLN	A	139	43.900	-3.456	55.504	1.00	51.66	C
ATOM	960	CB	GLN	A	139	44.336	-2.901	56.834	1.00	50.89	C
ATOM	961	CG	GLN	A	139	43.192	-3.002	57.796	1.00	49.04	C
ATOM	962	CD	GLN	A	139	42.872	-4.436	58.174	1.00	47.75	C
ATOM	963	OE1	GLN	A	139	42.017	-5.086	57.556	1.00	46.59	O
ATOM	964	NE2	GLN	A	139	43.568	-4.939	59.183	1.00	47.12	N
ATOM	965	C	GLN	A	139	44.442	-2.680	54.358	1.00	52.56	C
ATOM	966	O	GLN	A	139	43.921	-1.612	54.029	1.00	52.93	O
ATOM	967	N	GLU	A	140	45.447	-3.238	53.701	1.00	53.67	N
ATOM	968	CA	GLU	A	140	45.844	-2.693	52.406	1.00	54.76	C
ATOM	969	CB	GLU	A	140	47.351	-2.773	52.162	1.00	55.47	C
ATOM	970	CG	GLU	A	140	47.946	-1.439	51.737	1.00	58.88	C
ATOM	971	CD	GLU	A	140	48.860	-1.607	50.540	1.00	65.14	C
ATOM	972	OE1	GLU	A	140	50.058	-1.968	50.762	1.00	67.80	O
ATOM	973	OE2	GLU	A	140	48.375	-1.409	49.385	1.00	66.34	O
ATOM	974	C	GLU	A	140	45.024	-3.296	51.269	1.00	54.10	C
ATOM	975	O	GLU	A	140	44.977	-4.513	51.072	1.00	53.49	O
ATOM	976	N	CYS	A	141	44.359	-2.393	50.567	1.00	53.68	N
ATOM	977	CA	CYS	A	141	43.439	-2.703	49.509	1.00	53.83	C
ATOM	978	CB	CYS	A	141	42.013	-2.413	49.986	1.00	54.50	C
ATOM	979	SG	CYS	A	141	40.960	-3.782	50.545	1.00	57.49	S
ATOM	980	C	CYS	A	141	43.790	-1.723	48.390	1.00	53.22	C
ATOM	981	O	CYS	A	141	44.035	-0.549	48.631	1.00	53.34	O
ATOM	982	N	LEU	A	142	43.827	-2.184	47.156	1.00	52.38	N
ATOM	983	CA	LEU	A	142	44.056	-1.243	46.095	1.00	51.58	C
ATOM	984	CB	LEU	A	142	45.440	-1.465	45.508	1.00	51.42	C
ATOM	985	CG	LEU	A	142	46.580	-1.625	46.505	1.00	50.29	C
ATOM	986	CD1	LEU	A	142	47.110	-3.026	46.368	1.00	50.53	C
ATOM	987	CD2	LEU	A	142	47.667	-0.616	46.264	1.00	47.78	C
ATOM	988	C	LEU	A	142	42.942	-1.300	45.037	1.00	51.68	C
ATOM	989	O	LEU	A	142	42.503	-2.389	44.617	1.00	52.12	O
ATOM	990	N	LEU	A	143	42.466	-0.115	44.652	1.00	50.88	N
ATOM	991	CA	LEU	A	143	41.574	0.088	43.514	1.00	50.08	C
ATOM	992	CB	LEU	A	143	41.236	1.593	43.447	1.00	50.11	C
ATOM	993	CG	LEU	A	143	39.868	2.272	43.627	1.00	48.74	C
ATOM	994	CD1	LEU	A	143	39.110	1.656	44.757	1.00	48.23	C
ATOM	995	CD2	LEU	A	143	40.035	3.753	43.896	1.00	46.55	C
ATOM	996	C	LEU	A	143	42.375	-0.227	42.262	1.00	49.77	C
ATOM	997	O	LEU	A	143	43.568	0.057	42.247	1.00	49.73	O
ATOM	998	N	LEU	A	144	41.764	-0.767	41.201	1.00	49.16	N
ATOM	999	CA	LEU	A	144	42.482	-0.775	39.923	1.00	48.58	C
ATOM	1000	CB	LEU	A	144	41.696	-1.407	38.759	1.00	48.62	C
ATOM	1001	CG	LEU	A	144	42.485	-1.737	37.454	1.00	49.03	C
ATOM	1002	CD1	LEU	A	144	41.914	-2.933	36.732	1.00	49.65	C
ATOM	1003	CD2	LEU	A	144	42.581	-0.607	36.413	1.00	47.70	C
ATOM	1004	C	LEU	A	144	42.986	0.634	39.554	1.00	48.19	C
ATOM	1005	O	LEU	A	144	43.853	0.740	38.704	1.00	47.84	O

219/396

Figure 3A-19

ATOM	1006	N	GLU	A	145	42.469	1.700	40.180	1.00	47.90	N
ATOM	1007	CA	GLU	A	145	43.051	3.041	39.979	1.00	48.34	C
ATOM	1008	CB	GLU	A	145	42.466	3.725	38.743	1.00	48.01	C
ATOM	1009	CG	GLU	A	145	42.631	5.239	38.723	1.00	47.75	C
ATOM	1010	CD	GLU	A	145	43.899	5.726	38.024	1.00	49.16	C
ATOM	1011	OE1	GLU	A	145	44.519	4.949	37.230	1.00	49.51	O
ATOM	1012	OE2	GLU	A	145	44.271	6.910	38.263	1.00	48.27	O
ATOM	1013	C	GLU	A	145	42.981	4.017	41.179	1.00	48.95	C
ATOM	1014	O	GLU	A	145	41.877	4.281	41.682	1.00	49.81	O
ATOM	1015	N	PRO	A	146	44.133	4.558	41.637	1.00	48.70	N
ATOM	1016	CA	PRO	A	146	45.462	4.123	41.188	1.00	47.60	C
ATOM	1017	CB	PRO	A	146	46.302	5.372	41.344	1.00	47.50	C
ATOM	1018	CG	PRO	A	146	45.634	6.123	42.529	1.00	48.43	C
ATOM	1019	CD	PRO	A	146	44.222	5.641	42.646	1.00	48.60	C
ATOM	1020	C	PRO	A	146	45.928	3.113	42.168	1.00	46.94	C
ATOM	1021	O	PRO	A	146	45.651	3.251	43.351	1.00	46.99	O
ATOM	1022	N	GLY	A	147	46.615	2.103	41.696	1.00	46.57	N
ATOM	1023	CA	GLY	A	147	47.115	1.074	42.575	1.00	46.97	C
ATOM	1024	C	GLY	A	147	47.477	-0.018	41.623	1.00	47.42	C
ATOM	1025	O	GLY	A	147	48.396	0.157	40.832	1.00	47.86	O
ATOM	1026	N	LEU	A	148	46.736	-1.120	41.648	1.00	47.47	N
ATOM	1027	CA	LEU	A	148	46.924	-2.172	40.668	1.00	47.73	C
ATOM	1028	CB	LEU	A	148	45.598	-2.858	40.380	1.00	48.12	C
ATOM	1029	CG	LEU	A	148	45.173	-3.958	41.350	1.00	48.67	C
ATOM	1030	CD1	LEU	A	148	45.827	-3.809	42.702	1.00	49.25	C
ATOM	1031	CD2	LEU	A	148	43.678	-3.905	41.496	1.00	50.53	C
ATOM	1032	C	LEU	A	148	47.555	-1.639	39.377	1.00	47.79	C
ATOM	1033	O	LEU	A	148	48.479	-2.230	38.863	1.00	48.03	O
ATOM	1034	N	ASN	A	149	47.088	-0.507	38.868	1.00	47.98	N
ATOM	1035	CA	ASN	A	149	47.745	0.094	37.709	1.00	48.34	C
ATOM	1036	CB	ASN	A	149	46.955	1.263	37.077	1.00	49.67	C
ATOM	1037	CG	ASN	A	149	46.067	0.821	35.839	1.00	52.96	C
ATOM	1038	OD1	ASN	A	149	45.351	1.673	35.251	1.00	55.86	O
ATOM	1039	ND2	ASN	A	149	46.122	-0.489	35.451	1.00	53.56	N
ATOM	1040	C	ASN	A	149	49.189	0.457	37.984	1.00	47.08	C
ATOM	1041	O	ASN	A	149	50.054	-0.170	37.410	1.00	47.28	O
ATOM	1042	N	ALA	A	150	49.473	1.419	38.862	1.00	45.92	N
ATOM	1043	CA	ALA	A	150	50.886	1.751	39.160	1.00	44.93	C
ATOM	1044	CB	ALA	A	150	51.038	2.691	40.360	1.00	44.86	C
ATOM	1045	C	ALA	A	150	51.802	0.507	39.274	1.00	44.44	C
ATOM	1046	O	ALA	A	150	52.810	0.447	38.560	1.00	44.13	O
ATOM	1047	N	ILE	A	151	51.434	-0.482	40.111	1.00	43.58	N
ATOM	1048	CA	ILE	A	151	52.070	-1.804	40.111	1.00	42.82	C
ATOM	1049	CB	ILE	A	151	51.241	-2.807	40.853	1.00	42.55	C
ATOM	1050	CG1	ILE	A	151	51.225	-2.505	42.344	1.00	42.64	C
ATOM	1051	CD1	ILE	A	151	50.187	-3.408	43.101	1.00	43.31	C
ATOM	1052	CG2	ILE	A	151	51.729	-4.256	40.551	1.00	42.21	C
ATOM	1053	C	ILE	A	151	52.257	-2.320	38.687	1.00	43.33	C
ATOM	1054	O	ILE	A	151	53.362	-2.257	38.177	1.00	43.92	O
ATOM	1055	N	MET	A	152	51.191	-2.815	38.041	1.00	43.76	N
ATOM	1056	CA	MET	A	152	51.226	-3.311	36.643	1.00	44.14	C
ATOM	1057	CB	MET	A	152	49.811	-3.548	36.106	1.00	43.89	C
ATOM	1058	CG	MET	A	152	49.020	-4.627	36.749	1.00	43.52	C
ATOM	1059	SD	MET	A	152	50.079	-6.005	36.833	1.00	46.51	S
ATOM	1060	CE	MET	A	152	49.293	-7.261	35.835	1.00	45.90	C
ATOM	1061	C	MET	A	152	51.922	-2.373	35.651	1.00	44.99	C

220/396

Figure 3A-20

ATOM	1062	O	MET	A	152	52.028	-2.687	34.483	1.00	44.60	O
ATOM	1063	N	ALA	A	153	52.371	-1.215	36.121	1.00	46.36	N
ATOM	1064	CA	ALA	A	153	52.919	-0.188	35.258	1.00	47.91	C
ATOM	1065	CB	ALA	A	153	52.060	1.044	35.325	1.00	48.37	C
ATOM	1066	C	ALA	A	153	54.332	0.180	35.643	1.00	49.20	C
ATOM	1067	O	ALA	A	153	55.045	0.797	34.827	1.00	49.83	O
ATOM	1068	N	ASN	A	154	54.731	-0.137	36.884	1.00	50.11	N
ATOM	1069	CA	ASN	A	154	56.137	0.051	37.311	1.00	51.12	C
ATOM	1070	CB	ASN	A	154	56.419	1.484	37.802	1.00	51.46	C
ATOM	1071	CG	ASN	A	154	55.212	2.400	37.718	1.00	53.23	C
ATOM	1072	OD1	ASN	A	154	54.564	2.673	38.753	1.00	56.36	O
ATOM	1073	ND2	ASN	A	154	54.919	2.920	36.499	1.00	53.08	N
ATOM	1074	C	ASN	A	154	56.790	-0.959	38.279	1.00	51.27	C
ATOM	1075	O	ASN	A	154	57.992	-0.832	38.572	1.00	51.60	O
ATOM	1076	N	SER	A	155	56.022	-1.928	38.785	1.00	51.34	N
ATOM	1077	CA	SER	A	155	56.597	-3.007	39.562	1.00	51.45	C
ATOM	1078	CB	SER	A	155	55.543	-3.960	40.102	1.00	51.53	C
ATOM	1079	OG	SER	A	155	56.067	-5.269	40.317	1.00	49.42	O
ATOM	1080	C	SER	A	155	57.448	-3.760	38.585	1.00	52.45	C
ATOM	1081	O	SER	A	155	57.139	-3.796	37.375	1.00	51.75	O
ATOM	1082	N	LEU	A	156	58.532	-4.327	39.136	1.00	53.85	N
ATOM	1083	CA	LEU	A	156	59.503	-5.187	38.425	1.00	54.43	C
ATOM	1084	CB	LEU	A	156	60.901	-4.555	38.356	1.00	54.16	C
ATOM	1085	CG	LEU	A	156	61.041	-3.480	37.281	1.00	54.38	C
ATOM	1086	CD1	LEU	A	156	60.570	-2.106	37.774	1.00	54.35	C
ATOM	1087	CD2	LEU	A	156	62.473	-3.404	36.809	1.00	55.90	C
ATOM	1088	C	LEU	A	156	59.564	-6.540	39.114	1.00	54.66	C
ATOM	1089	O	LEU	A	156	59.792	-7.561	38.475	1.00	54.70	O
ATOM	1090	N	ASP	A	157	59.325	-6.538	40.416	1.00	54.97	N
ATOM	1091	CA	ASP	A	157	59.213	-7.774	41.155	1.00	55.94	C
ATOM	1092	CB	ASP	A	157	58.720	-7.442	42.569	1.00	57.06	C
ATOM	1093	CG	ASP	A	157	59.479	-8.200	43.662	1.00	60.28	C
ATOM	1094	OD1	ASP	A	157	60.006	-7.491	44.581	1.00	62.19	O
ATOM	1095	OD2	ASP	A	157	59.583	-9.475	43.679	1.00	62.77	O
ATOM	1096	C	ASP	A	157	58.232	-8.759	40.500	1.00	55.19	C
ATOM	1097	O	ASP	A	157	57.077	-8.818	40.907	1.00	55.34	O
ATOM	1098	N	TYR	A	158	58.665	-9.527	39.500	1.00	54.31	N
ATOM	1099	CA	TYR	A	158	57.791	-10.529	38.879	1.00	53.88	C
ATOM	1100	CB	TYR	A	158	58.593	-11.773	38.522	1.00	52.56	C
ATOM	1101	CG	TYR	A	158	57.768	-12.881	37.926	1.00	50.09	C
ATOM	1102	CD1	TYR	A	158	57.806	-13.154	36.552	1.00	47.96	C
ATOM	1103	CE1	TYR	A	158	57.041	-14.187	35.971	1.00	45.47	C
ATOM	1104	CZ	TYR	A	158	56.233	-14.957	36.772	1.00	46.42	C
ATOM	1105	OH	TYR	A	158	55.458	-15.981	36.244	1.00	43.95	O
ATOM	1106	CE2	TYR	A	158	56.194	-14.706	38.152	1.00	49.61	C
ATOM	1107	CD2	TYR	A	158	56.950	-13.663	38.719	1.00	49.16	C
ATOM	1108	C	TYR	A	158	56.584	-10.894	39.796	1.00	54.90	C
ATOM	1109	O	TYR	A	158	55.398	-10.707	39.463	1.00	55.46	O
ATOM	1110	N	ASN	A	159	56.899	-11.399	40.970	1.00	55.51	N
ATOM	1111	CA	ASN	A	159	55.900	-11.609	42.001	1.00	55.94	C
ATOM	1112	CB	ASN	A	159	56.633	-11.823	43.323	1.00	56.45	C
ATOM	1113	CG	ASN	A	159	57.305	-13.139	43.355	1.00	57.25	C
ATOM	1114	OD1	ASN	A	159	56.642	-14.165	43.536	1.00	58.79	O
ATOM	1115	ND2	ASN	A	159	58.611	-13.150	43.085	1.00	57.83	N
ATOM	1116	C	ASN	A	159	54.779	-10.558	42.147	1.00	55.36	C
ATOM	1117	O	ASN	A	159	53.605	-10.907	42.159	1.00	55.38	O

221/396

Figure 3A-21

ATOM	1118	N	GLU	A	160	55.144	-9.289	42.294	1.00	54.91	N
ATOM	1119	CA	GLU	A	160	54.157	-8.222	42.465	1.00	54.51	C
ATOM	1120	CB	GLU	A	160	54.826	-6.848	42.627	1.00	54.58	C
ATOM	1121	CG	GLU	A	160	53.957	-5.757	43.235	1.00	54.97	C
ATOM	1122	CD	GLU	A	160	54.742	-4.468	43.497	1.00	57.62	C
ATOM	1123	OE1	GLU	A	160	54.366	-3.660	44.389	1.00	58.01	O
ATOM	1124	OE2	GLU	A	160	55.755	-4.244	42.801	1.00	60.09	O
ATOM	1125	C	GLU	A	160	53.303	-8.257	41.211	1.00	53.94	C
ATOM	1126	O	GLU	A	160	52.156	-8.751	41.259	1.00	54.54	O
ATOM	1127	N	ARG	A	161	53.866	-7.770	40.095	1.00	51.93	N
ATOM	1128	CA	ARG	A	161	53.214	-7.873	38.804	1.00	49.77	C
ATOM	1129	CB	ARG	A	161	54.252	-8.035	37.703	1.00	49.60	C
ATOM	1130	CG	ARG	A	161	55.220	-6.882	37.613	1.00	47.56	C
ATOM	1131	CD	ARG	A	161	54.636	-5.643	37.013	1.00	44.02	C
ATOM	1132	NE	ARG	A	161	54.128	-5.907	35.680	1.00	40.32	N
ATOM	1133	CZ	ARG	A	161	54.699	-5.465	34.600	1.00	38.89	C
ATOM	1134	NH1	ARG	A	161	55.792	-4.732	34.704	1.00	39.66	N
ATOM	1135	NH2	ARG	A	161	54.181	-5.745	33.421	1.00	37.80	N
ATOM	1136	C	ARG	A	161	52.279	-9.073	38.821	1.00	48.96	C
ATOM	1137	O	ARG	A	161	51.089	-8.963	38.504	1.00	48.66	O
ATOM	1138	N	LEU	A	162	52.810	-10.208	39.246	1.00	47.90	N
ATOM	1139	CA	LEU	A	162	51.993	-11.387	39.346	1.00	47.52	C
ATOM	1140	CB	LEU	A	162	52.811	-12.581	39.779	1.00	47.26	C
ATOM	1141	CG	LEU	A	162	52.364	-13.714	38.893	1.00	47.70	C
ATOM	1142	CD1	LEU	A	162	53.343	-14.758	39.090	1.00	50.55	C
ATOM	1143	CD2	LEU	A	162	50.986	-14.245	39.263	1.00	47.97	C
ATOM	1144	C	LEU	A	162	50.683	-11.242	40.160	1.00	47.27	C
ATOM	1145	O	LEU	A	162	49.616	-11.404	39.579	1.00	47.72	O
ATOM	1146	N	TRP	A	163	50.737	-10.937	41.461	1.00	46.67	N
ATOM	1147	CA	TRP	A	163	49.508	-10.911	42.272	1.00	46.18	C
ATOM	1148	CB	TRP	A	163	49.792	-10.730	43.789	1.00	46.37	C
ATOM	1149	CG	TRP	A	163	48.625	-10.249	44.698	1.00	47.00	C
ATOM	1150	CD1	TRP	A	163	47.636	-11.018	45.317	1.00	46.88	C
ATOM	1151	NE1	TRP	A	163	46.791	-10.208	46.043	1.00	44.97	N
ATOM	1152	CE2	TRP	A	163	47.230	-8.913	45.933	1.00	47.15	C
ATOM	1153	CD2	TRP	A	163	48.380	-8.907	45.102	1.00	47.01	C
ATOM	1154	CE3	TRP	A	163	49.006	-7.680	44.827	1.00	48.13	C
ATOM	1155	CZ3	TRP	A	163	48.494	-6.519	45.358	1.00	48.61	C
ATOM	1156	CH2	TRP	A	163	47.361	-6.554	46.174	1.00	51.35	C
ATOM	1157	CZ2	TRP	A	163	46.707	-7.748	46.470	1.00	50.07	C
ATOM	1158	C	TRP	A	163	48.501	-9.913	41.678	1.00	45.90	C
ATOM	1159	O	TRP	A	163	47.403	-10.312	41.242	1.00	45.41	O
ATOM	1160	N	ALA	A	164	48.887	-8.643	41.571	1.00	45.54	N
ATOM	1161	CA	ALA	A	164	48.034	-7.670	40.864	1.00	45.09	C
ATOM	1162	CB	ALA	A	164	48.843	-6.471	40.277	1.00	44.53	C
ATOM	1163	C	ALA	A	164	47.290	-8.426	39.772	1.00	44.45	C
ATOM	1164	O	ALA	A	164	46.066	-8.561	39.840	1.00	44.18	O
ATOM	1165	N	TRP	A	165	48.046	-8.985	38.823	1.00	43.76	N
ATOM	1166	CA	TRP	A	165	47.455	-9.583	37.641	1.00	43.37	C
ATOM	1167	CB	TRP	A	165	48.488	-10.323	36.808	1.00	42.45	C
ATOM	1168	CG	TRP	A	165	47.951	-10.730	35.464	1.00	38.24	C
ATOM	1169	CD1	TRP	A	165	48.152	-10.095	34.298	1.00	36.11	C
ATOM	1170	NE1	TRP	A	165	47.519	-10.756	33.276	1.00	33.73	N
ATOM	1171	CE2	TRP	A	165	46.868	-11.836	33.793	1.00	31.19	C
ATOM	1172	CD2	TRP	A	165	47.113	-11.848	35.169	1.00	32.98	C
ATOM	1173	CE3	TRP	A	165	46.538	-12.857	35.934	1.00	32.24	C

222/396

Figure 3A-22

ATOM	1174	CZ3	TRP	A	165	45.769	-13.786	35.310	1.00	32.57	C
ATOM	1175	CH2	TRP	A	165	45.545	-13.745	33.924	1.00	30.48	C
ATOM	1176	CZ2	TRP	A	165	46.084	-12.778	33.162	1.00	30.23	C
ATOM	1177	C	TRP	A	165	46.261	-10.500	37.912	1.00	44.44	C
ATOM	1178	O	TRP	A	165	45.238	-10.389	37.220	1.00	45.15	O
ATOM	1179	N	GLU	A	166	46.392	-11.416	38.872	1.00	44.68	N
ATOM	1180	CA	GLU	A	166	45.359	-12.422	39.115	1.00	45.03	C
ATOM	1181	CB	GLU	A	166	46.005	-13.697	39.628	1.00	45.44	C
ATOM	1182	CG	GLU	A	166	45.019	-14.707	40.199	1.00	47.52	C
ATOM	1183	CD	GLU	A	166	44.506	-15.635	39.118	1.00	49.71	C
ATOM	1184	OE1	GLU	A	166	44.909	-15.415	37.940	1.00	49.55	O
ATOM	1185	OE2	GLU	A	166	43.730	-16.571	39.457	1.00	49.35	O
ATOM	1186	C	GLU	A	166	44.347	-11.889	40.124	1.00	44.92	C
ATOM	1187	O	GLU	A	166	43.120	-11.949	39.908	1.00	43.84	O
ATOM	1188	N	SER	A	167	44.907	-11.408	41.243	1.00	45.08	N
ATOM	1189	CA	SER	A	167	44.267	-10.471	42.172	1.00	45.00	C
ATOM	1190	CB	SER	A	167	45.203	-9.261	42.375	1.00	45.44	C
ATOM	1191	OG	SER	A	167	45.736	-9.152	43.684	1.00	47.54	O
ATOM	1192	C	SER	A	167	42.960	-9.942	41.604	1.00	43.88	C
ATOM	1193	O	SER	A	167	41.896	-10.430	41.954	1.00	43.49	O
ATOM	1194	N	TRP	A	168	43.105	-8.945	40.718	1.00	42.73	N
ATOM	1195	CA	TRP	A	168	42.032	-8.247	40.043	1.00	41.46	C
ATOM	1196	CB	TRP	A	168	42.588	-7.105	39.209	1.00	40.70	C
ATOM	1197	CG	TRP	A	168	41.564	-6.341	38.367	1.00	37.89	C
ATOM	1198	CD1	TRP	A	168	41.369	-6.453	37.039	1.00	36.29	C
ATOM	1199	NE1	TRP	A	168	40.393	-5.586	36.613	1.00	34.87	N
ATOM	1200	CE2	TRP	A	168	39.941	-4.881	37.687	1.00	34.91	C
ATOM	1201	CD2	TRP	A	168	40.649	-5.331	38.809	1.00	35.70	C
ATOM	1202	CE3	TRP	A	168	40.360	-4.752	40.046	1.00	35.61	C
ATOM	1203	CZ3	TRP	A	168	39.392	-3.787	40.122	1.00	34.08	C
ATOM	1204	CH2	TRP	A	168	38.714	-3.368	38.997	1.00	35.04	C
ATOM	1205	CZ2	TRP	A	168	38.975	-3.896	37.764	1.00	35.30	C
ATOM	1206	C	TRP	A	168	41.231	-9.165	39.161	1.00	41.61	C
ATOM	1207	O	TRP	A	168	40.017	-9.028	39.101	1.00	42.03	O
ATOM	1208	N	ARG	A	169	41.875	-10.101	38.481	1.00	41.57	N
ATOM	1209	CA	ARG	A	169	41.098	-11.000	37.648	1.00	42.22	C
ATOM	1210	CB	ARG	A	169	41.974	-11.768	36.655	1.00	41.59	C
ATOM	1211	CG	ARG	A	169	41.925	-11.278	35.209	1.00	37.94	C
ATOM	1212	CD	ARG	A	169	43.178	-11.656	34.436	1.00	31.40	C
ATOM	1213	NE	ARG	A	169	43.453	-10.959	33.167	1.00	25.73	N
ATOM	1214	CZ	ARG	A	169	43.820	-9.681	33.039	1.00	21.91	C
ATOM	1215	NH1	ARG	A	169	44.089	-9.206	31.823	1.00	19.41	N
ATOM	1216	NH2	ARG	A	169	43.916	-8.885	34.110	1.00	18.15	N
ATOM	1217	C	ARG	A	169	40.308	-11.945	38.562	1.00	44.02	C
ATOM	1218	O	ARG	A	169	39.194	-12.378	38.202	1.00	43.99	O
ATOM	1219	N	SER	A	170	40.881	-12.237	39.743	1.00	45.73	N
ATOM	1220	CA	SER	A	170	40.253	-13.120	40.744	1.00	47.43	C
ATOM	1221	CB	SER	A	170	41.325	-13.795	41.601	1.00	47.15	C
ATOM	1222	OG	SER	A	170	41.139	-13.558	42.989	1.00	47.26	O
ATOM	1223	C	SER	A	170	39.193	-12.419	41.636	1.00	48.91	C
ATOM	1224	O	SER	A	170	38.002	-12.789	41.635	1.00	49.54	O
ATOM	1225	N	GLU	A	171	39.625	-11.424	42.410	1.00	50.06	N
ATOM	1226	CA	GLU	A	171	38.696	-10.643	43.209	1.00	50.80	C
ATOM	1227	CB	GLU	A	171	39.416	-9.540	43.986	1.00	51.22	C
ATOM	1228	CG	GLU	A	171	39.835	-9.971	45.396	1.00	53.80	C
ATOM	1229	CD	GLU	A	171	40.902	-11.077	45.440	1.00	56.50	C

223/396

Figure 3A-23

ATOM	1230	OE1	GLU	A	171	42.104	-10.723	45.320	1.00	57.51	O
ATOM	1231	OE2	GLU	A	171	40.546	-12.289	45.618	1.00	56.93	O
ATOM	1232	C	GLU	A	171	37.608	-10.103	42.299	1.00	50.72	C
ATOM	1233	O	GLU	A	171	36.494	-10.655	42.314	1.00	51.24	O
ATOM	1234	N	VAL	A	172	37.917	-9.097	41.476	1.00	50.13	N
ATOM	1235	CA	VAL	A	172	36.873	-8.513	40.625	1.00	50.21	C
ATOM	1236	CB	VAL	A	172	37.127	-7.030	40.234	1.00	50.26	C
ATOM	1237	CG1	VAL	A	172	37.965	-6.337	41.266	1.00	49.91	C
ATOM	1238	CG2	VAL	A	172	37.715	-6.919	38.840	1.00	50.27	C
ATOM	1239	C	VAL	A	172	36.449	-9.345	39.398	1.00	50.07	C
ATOM	1240	O	VAL	A	172	35.332	-9.825	39.337	1.00	49.92	O
ATOM	1241	N	GLY	A	173	37.324	-9.500	38.424	1.00	50.04	N
ATOM	1242	CA	GLY	A	173	36.972	-10.183	37.197	1.00	50.77	C
ATOM	1243	C	GLY	A	173	35.967	-11.315	37.304	1.00	51.25	C
ATOM	1244	O	GLY	A	173	35.145	-11.479	36.413	1.00	51.38	O
ATOM	1245	N	LYS	A	174	36.044	-12.094	38.382	1.00	51.88	N
ATOM	1246	CA	LYS	A	174	35.116	-13.200	38.652	1.00	52.33	C
ATOM	1247	CB	LYS	A	174	35.544	-13.967	39.897	1.00	52.24	C
ATOM	1248	CG	LYS	A	174	35.950	-15.389	39.642	1.00	52.92	C
ATOM	1249	CD	LYS	A	174	37.448	-15.598	39.833	1.00	54.74	C
ATOM	1250	CE	LYS	A	174	37.746	-16.413	41.089	1.00	56.21	C
ATOM	1251	NZ	LYS	A	174	38.443	-17.711	40.776	1.00	57.57	N
ATOM	1252	C	LYS	A	174	33.715	-12.678	38.884	1.00	52.77	C
ATOM	1253	O	LYS	A	174	32.756	-13.207	38.326	1.00	53.25	O
ATOM	1254	N	GLN	A	175	33.616	-11.640	39.719	1.00	53.03	N
ATOM	1255	CA	GLN	A	175	32.357	-10.971	40.077	1.00	53.23	C
ATOM	1256	CB	GLN	A	175	32.666	-9.664	40.833	1.00	53.93	C
ATOM	1257	CG	GLN	A	175	32.689	-9.715	42.397	1.00	56.74	C
ATOM	1258	CD	GLN	A	175	33.152	-8.383	43.033	1.00	59.17	C
ATOM	1259	OE1	GLN	A	175	32.321	-7.582	43.500	1.00	59.27	O
ATOM	1260	NE2	GLN	A	175	34.474	-8.148	43.038	1.00	58.89	N
ATOM	1261	C	GLN	A	175	31.568	-10.610	38.832	1.00	52.39	C
ATOM	1262	O	GLN	A	175	30.328	-10.531	38.843	1.00	51.82	O
ATOM	1263	N	LEU	A	176	32.325	-10.372	37.766	1.00	51.75	N
ATOM	1264	CA	LEU	A	176	31.768	-9.903	36.527	1.00	51.32	C
ATOM	1265	CB	LEU	A	176	32.865	-9.370	35.590	1.00	50.41	C
ATOM	1266	CG	LEU	A	176	33.308	-7.907	35.546	1.00	47.68	C
ATOM	1267	CD1	LEU	A	176	32.195	-6.912	35.463	1.00	45.13	C
ATOM	1268	CD2	LEU	A	176	34.094	-7.657	36.765	1.00	48.19	C
ATOM	1269	C	LEU	A	176	30.977	-11.027	35.875	1.00	51.84	C
ATOM	1270	O	LEU	A	176	29.785	-10.874	35.611	1.00	52.26	O
ATOM	1271	N	ARG	A	177	31.628	-12.158	35.653	1.00	52.05	N
ATOM	1272	CA	ARG	A	177	31.094	-13.193	34.782	1.00	52.81	C
ATOM	1273	CB	ARG	A	177	31.656	-14.557	35.170	1.00	53.24	C
ATOM	1274	CG	ARG	A	177	31.445	-15.619	34.111	1.00	53.52	C
ATOM	1275	CD	ARG	A	177	32.612	-15.736	33.167	1.00	52.25	C
ATOM	1276	NE	ARG	A	177	32.350	-16.453	31.924	1.00	50.95	N
ATOM	1277	CZ	ARG	A	177	31.775	-17.643	31.822	1.00	51.37	C
ATOM	1278	NH1	ARG	A	177	31.655	-18.169	30.617	1.00	51.14	N
ATOM	1279	NH2	ARG	A	177	31.300	-18.298	32.895	1.00	52.29	N
ATOM	1280	C	ARG	A	177	29.570	-13.271	34.698	1.00	53.34	C
ATOM	1281	O	ARG	A	177	29.018	-13.011	33.627	1.00	52.96	O
ATOM	1282	N	PRO	A	178	28.907	-13.632	35.813	1.00	54.02	N
ATOM	1283	CA	PRO	A	178	27.458	-13.950	35.840	1.00	54.39	C
ATOM	1284	CB	PRO	A	178	27.159	-13.990	37.335	1.00	54.74	C
ATOM	1285	CG	PRO	A	178	28.450	-14.547	37.910	1.00	54.62	C

224/396

Figure 3A-24

ATOM	1286	CD	PRO	A	178	29.498	-13.761	37.161	1.00	53.92	C
ATOM	1287	C	PRO	A	178	26.545	-12.942	35.158	1.00	54.28	C
ATOM	1288	O	PRO	A	178	25.663	-13.318	34.385	1.00	53.81	O
ATOM	1289	N	LEU	A	179	26.780	-11.674	35.465	1.00	54.55	N
ATOM	1290	CA	LEU	A	179	26.252	-10.553	34.698	1.00	55.00	C
ATOM	1291	CB	LEU	A	179	26.701	-9.214	35.307	1.00	55.31	C
ATOM	1292	CG	LEU	A	179	26.587	-9.025	36.824	1.00	56.71	C
ATOM	1293	CD1	LEU	A	179	27.970	-8.663	37.437	1.00	58.00	C
ATOM	1294	CD2	LEU	A	179	25.515	-8.000	37.192	1.00	56.28	C
ATOM	1295	C	LEU	A	179	26.723	-10.571	33.259	1.00	54.66	C
ATOM	1296	O	LEU	A	179	26.008	-10.101	32.382	1.00	54.70	O
ATOM	1297	N	TYR	A	180	27.938	-11.061	33.014	1.00	54.46	N
ATOM	1298	CA	TYR	A	180	28.510	-10.884	31.679	1.00	54.44	C
ATOM	1299	CB	TYR	A	180	30.042	-11.131	31.560	1.00	54.15	C
ATOM	1300	CG	TYR	A	180	30.497	-10.571	30.236	1.00	51.76	C
ATOM	1301	CD1	TYR	A	180	30.347	-9.214	29.964	1.00	51.00	C
ATOM	1302	CE1	TYR	A	180	30.687	-8.666	28.726	1.00	49.16	C
ATOM	1303	CZ	TYR	A	180	31.155	-9.481	27.741	1.00	47.34	C
ATOM	1304	OH	TYR	A	180	31.501	-8.921	26.538	1.00	45.37	O
ATOM	1305	CE2	TYR	A	180	31.283	-10.846	27.977	1.00	48.63	C
ATOM	1306	CD2	TYR	A	180	30.937	-11.386	29.221	1.00	49.10	C
ATOM	1307	C	TYR	A	180	27.723	-11.649	30.630	1.00	54.82	C
ATOM	1308	O	TYR	A	180	27.252	-11.046	29.635	1.00	54.57	O
ATOM	1309	N	GLU	A	181	27.594	-12.966	30.877	1.00	54.87	N
ATOM	1310	CA	GLU	A	181	26.662	-13.842	30.168	1.00	54.66	C
ATOM	1311	CB	GLU	A	181	26.320	-15.094	30.996	1.00	54.78	C
ATOM	1312	CG	GLU	A	181	27.166	-15.338	32.251	1.00	56.33	C
ATOM	1313	CD	GLU	A	181	28.016	-16.620	32.200	1.00	58.23	C
ATOM	1314	OE1	GLU	A	181	27.543	-17.722	32.609	1.00	57.48	O
ATOM	1315	OE2	GLU	A	181	29.185	-16.521	31.757	1.00	59.25	O
ATOM	1316	C	GLU	A	181	25.414	-13.019	29.874	1.00	54.35	C
ATOM	1317	O	GLU	A	181	25.350	-12.361	28.822	1.00	54.14	O
ATOM	1318	N	GLU	A	182	24.465	-13.000	30.820	1.00	53.83	N
ATOM	1319	CA	GLU	A	182	23.310	-12.097	30.769	1.00	53.52	C
ATOM	1320	CB	GLU	A	182	23.223	-11.316	32.058	1.00	53.66	C
ATOM	1321	CG	GLU	A	182	21.958	-11.569	32.803	1.00	57.36	C
ATOM	1322	CD	GLU	A	182	22.241	-12.351	34.058	1.00	62.39	C
ATOM	1323	OE1	GLU	A	182	21.813	-11.893	35.152	1.00	63.35	O
ATOM	1324	OE2	GLU	A	182	22.914	-13.412	33.943	1.00	65.23	O
ATOM	1325	C	GLU	A	182	23.343	-11.069	29.638	1.00	52.58	C
ATOM	1326	O	GLU	A	182	22.513	-11.103	28.756	1.00	52.31	O
ATOM	1327	N	TYR	A	183	24.327	-10.170	29.673	1.00	51.86	N
ATOM	1328	CA	TYR	A	183	24.316	-8.961	28.857	1.00	51.21	C
ATOM	1329	CB	TYR	A	183	25.277	-7.881	29.432	1.00	51.73	C
ATOM	1330	CG	TYR	A	183	26.169	-7.111	28.429	1.00	53.18	C
ATOM	1331	CD1	TYR	A	183	27.336	-7.698	27.875	1.00	53.45	C
ATOM	1332	CE1	TYR	A	183	28.159	-6.995	26.989	1.00	51.06	C
ATOM	1333	CZ	TYR	A	183	27.834	-5.707	26.653	1.00	50.99	C
ATOM	1334	OH	TYR	A	183	28.642	-5.019	25.794	1.00	51.69	O
ATOM	1335	CE2	TYR	A	183	26.703	-5.099	27.171	1.00	51.57	C
ATOM	1336	CD2	TYR	A	183	25.875	-5.795	28.061	1.00	52.73	C
ATOM	1337	C	TYR	A	183	24.585	-9.316	27.412	1.00	50.07	C
ATOM	1338	O	TYR	A	183	24.080	-8.643	26.496	1.00	49.74	O
ATOM	1339	N	VAL	A	184	25.366	-10.376	27.219	1.00	48.62	N
ATOM	1340	CA	VAL	A	184	25.491	-10.975	25.896	1.00	47.95	C
ATOM	1341	CB	VAL	A	184	26.718	-11.952	25.777	1.00	48.25	C

225/396

Figure 3A-25

ATOM	1342	CG1	VAL	A	184	27.883	-11.457	26.610	1.00	48.69	C
ATOM	1343	CG2	VAL	A	184	26.355	-13.420	26.132	1.00	47.89	C
ATOM	1344	C	VAL	A	184	24.178	-11.669	25.494	1.00	46.98	C
ATOM	1345	O	VAL	A	184	23.699	-11.502	24.383	1.00	46.89	O
ATOM	1346	N	VAL	A	185	23.591	-12.389	26.442	1.00	45.56	N
ATOM	1347	CA	VAL	A	185	22.476	-13.269	26.223	1.00	44.34	C
ATOM	1348	CB	VAL	A	185	22.487	-14.330	27.315	1.00	44.54	C
ATOM	1349	CG1	VAL	A	185	21.114	-14.570	27.938	1.00	44.15	C
ATOM	1350	CG2	VAL	A	185	23.103	-15.618	26.769	1.00	45.69	C
ATOM	1351	C	VAL	A	185	21.190	-12.506	26.223	1.00	43.82	C
ATOM	1352	O	VAL	A	185	20.198	-12.967	25.706	1.00	43.69	O
ATOM	1353	N	LEU	A	186	21.210	-11.338	26.836	1.00	44.16	N
ATOM	1354	CA	LEU	A	186	20.153	-10.337	26.694	1.00	44.69	C
ATOM	1355	CB	LEU	A	186	20.335	-9.207	27.724	1.00	44.82	C
ATOM	1356	CG	LEU	A	186	19.459	-8.817	28.913	1.00	44.18	C
ATOM	1357	CD1	LEU	A	186	17.961	-8.893	28.592	1.00	43.89	C
ATOM	1358	CD2	LEU	A	186	19.874	-9.667	30.121	1.00	43.21	C
ATOM	1359	C	LEU	A	186	20.431	-9.715	25.364	1.00	44.98	C
ATOM	1360	O	LEU	A	186	20.170	-10.298	24.327	1.00	44.26	O
ATOM	1361	N	LYS	A	187	21.017	-8.524	25.440	1.00	45.94	N
ATOM	1362	CA	LYS	A	187	21.526	-7.796	24.300	1.00	47.44	C
ATOM	1363	CB	LYS	A	187	22.901	-7.194	24.630	1.00	46.82	C
ATOM	1364	CG	LYS	A	187	23.144	-5.785	24.025	1.00	46.81	C
ATOM	1365	CD	LYS	A	187	23.190	-4.685	25.121	1.00	46.69	C
ATOM	1366	CE	LYS	A	187	24.319	-3.669	24.935	1.00	44.27	C
ATOM	1367	NZ	LYS	A	187	23.849	-2.265	24.977	1.00	43.10	N
ATOM	1368	C	LYS	A	187	21.499	-8.558	22.937	1.00	48.78	C
ATOM	1369	O	LYS	A	187	20.838	-8.075	21.985	1.00	48.39	O
ATOM	1370	N	ASN	A	188	22.178	-9.723	22.831	1.00	50.29	N
ATOM	1371	CA	ASN	A	188	22.194	-10.463	21.547	1.00	51.77	C
ATOM	1372	CB	ASN	A	188	22.833	-11.870	21.604	1.00	51.53	C
ATOM	1373	CG	ASN	A	188	24.162	-11.978	20.804	1.00	51.32	C
ATOM	1374	OD1	ASN	A	188	24.450	-11.175	19.914	1.00	50.21	O
ATOM	1375	ND2	ASN	A	188	24.970	-12.985	21.140	1.00	51.70	N
ATOM	1376	C	ASN	A	188	20.760	-10.533	21.082	1.00	53.11	C
ATOM	1377	O	ASN	A	188	20.468	-10.062	19.972	1.00	53.33	O
ATOM	1378	N	GLU	A	189	19.875	-11.059	21.955	1.00	54.63	N
ATOM	1379	CA	GLU	A	189	18.412	-10.941	21.799	1.00	55.96	C
ATOM	1380	CB	GLU	A	189	17.656	-11.287	23.091	1.00	56.06	C
ATOM	1381	CG	GLU	A	189	16.144	-11.041	23.015	1.00	59.32	C
ATOM	1382	CD	GLU	A	189	15.293	-12.148	23.666	1.00	63.62	C
ATOM	1383	OE1	GLU	A	189	14.869	-13.139	22.961	1.00	63.40	O
ATOM	1384	OE2	GLU	A	189	15.039	-12.012	24.899	1.00	64.93	O
ATOM	1385	C	GLU	A	189	18.011	-9.551	21.276	1.00	56.31	C
ATOM	1386	O	GLU	A	189	17.494	-9.442	20.161	1.00	56.47	O
ATOM	1387	N	MET	A	190	18.296	-8.504	22.056	1.00	56.87	N
ATOM	1388	CA	MET	A	190	17.981	-7.117	21.694	1.00	57.27	C
ATOM	1389	CB	MET	A	190	18.693	-6.164	22.647	1.00	57.23	C
ATOM	1390	CG	MET	A	190	18.359	-4.710	22.445	1.00	58.28	C
ATOM	1391	SD	MET	A	190	18.982	-3.871	20.926	1.00	62.38	S
ATOM	1392	CE	MET	A	190	20.799	-4.279	20.874	1.00	61.34	C
ATOM	1393	C	MET	A	190	18.233	-6.712	20.215	1.00	57.47	C
ATOM	1394	O	MET	A	190	17.403	-6.018	19.620	1.00	57.59	O
ATOM	1395	N	ALA	A	191	19.354	-7.119	19.619	1.00	57.67	N
ATOM	1396	CA	ALA	A	191	19.650	-6.716	18.218	1.00	57.65	C
ATOM	1397	CB	ALA	A	191	21.192	-6.467	17.970	1.00	57.78	C

226/396

Figure 3A-26

ATOM	1398	C	ALA	A	191	19.092	-7.653	17.153	1.00	57.20	C
ATOM	1399	O	ALA	A	191	18.796	-7.223	16.040	1.00	56.98	O
ATOM	1400	N	ARG	A	192	18.993	-8.938	17.470	1.00	56.93	N
ATOM	1401	CA	ARG	A	192	18.454	-9.870	16.501	1.00	57.09	C
ATOM	1402	CB	ARG	A	192	18.403	-11.300	17.050	1.00	57.31	C
ATOM	1403	CG	ARG	A	192	19.720	-11.915	17.559	1.00	59.03	C
ATOM	1404	CD	ARG	A	192	19.487	-12.892	18.735	1.00	64.46	C
ATOM	1405	NE	ARG	A	192	18.141	-12.684	19.323	1.00	68.29	N
ATOM	1406	CZ	ARG	A	192	17.320	-13.638	19.792	1.00	68.76	C
ATOM	1407	NH1	ARG	A	192	16.116	-13.292	20.277	1.00	67.15	N
ATOM	1408	NH2	ARG	A	192	17.694	-14.926	19.770	1.00	68.52	N
ATOM	1409	C	ARG	A	192	17.045	-9.366	16.176	1.00	56.59	C
ATOM	1410	O	ARG	A	192	16.680	-9.156	15.000	1.00	56.92	O
ATOM	1411	N	ALA	A	193	16.279	-9.134	17.243	1.00	55.47	N
ATOM	1412	CA	ALA	A	193	14.928	-8.624	17.144	1.00	53.89	C
ATOM	1413	CB	ALA	A	193	14.147	-8.914	18.422	1.00	53.68	C
ATOM	1414	C	ALA	A	193	15.005	-7.143	16.878	1.00	52.97	C
ATOM	1415	O	ALA	A	193	14.125	-6.410	17.291	1.00	52.65	O
ATOM	1416	N	ASN	A	194	16.069	-6.719	16.187	1.00	52.41	N
ATOM	1417	CA	ASN	A	194	16.257	-5.326	15.690	1.00	52.09	C
ATOM	1418	CB	ASN	A	194	17.104	-4.481	16.663	1.00	51.79	C
ATOM	1419	CG	ASN	A	194	16.652	-3.036	16.733	1.00	49.93	C
ATOM	1420	OD1	ASN	A	194	16.163	-2.460	15.748	1.00	47.07	O
ATOM	1421	ND2	ASN	A	194	16.819	-2.440	17.906	1.00	47.86	N
ATOM	1422	C	ASN	A	194	16.876	-5.305	14.280	1.00	52.09	C
ATOM	1423	O	ASN	A	194	17.091	-4.243	13.669	1.00	50.99	O
ATOM	1424	N	HIS	A	195	17.143	-6.526	13.819	1.00	52.70	N
ATOM	1425	CA	HIS	A	195	17.563	-6.904	12.472	1.00	53.57	C
ATOM	1426	CB	HIS	A	195	17.483	-5.763	11.451	1.00	54.16	C
ATOM	1427	CG	HIS	A	195	16.076	-5.305	11.213	1.00	58.94	C
ATOM	1428	ND1	HIS	A	195	15.764	-4.061	10.699	1.00	62.25	N
ATOM	1429	CE1	HIS	A	195	14.447	-3.932	10.636	1.00	63.95	C
ATOM	1430	NE2	HIS	A	195	13.891	-5.037	11.109	1.00	64.28	N
ATOM	1431	CD2	HIS	A	195	14.888	-5.915	11.473	1.00	62.26	C
ATOM	1432	C	HIS	A	195	18.902	-7.612	12.494	1.00	52.83	C
ATOM	1433	O	HIS	A	195	19.009	-8.750	12.033	1.00	53.08	O
ATOM	1434	N	TYR	A	196	19.901	-6.973	13.089	1.00	51.93	N
ATOM	1435	CA	TYR	A	196	21.270	-7.405	12.895	1.00	50.92	C
ATOM	1436	CB	TYR	A	196	22.224	-6.508	13.645	1.00	50.48	C
ATOM	1437	CG	TYR	A	196	22.150	-5.094	13.170	1.00	48.66	C
ATOM	1438	CD1	TYR	A	196	22.746	-4.715	11.973	1.00	46.37	C
ATOM	1439	CE1	TYR	A	196	22.664	-3.417	11.529	1.00	47.18	C
ATOM	1440	CZ	TYR	A	196	21.980	-2.468	12.281	1.00	47.13	C
ATOM	1441	OH	TYR	A	196	21.908	-1.168	11.823	1.00	48.13	O
ATOM	1442	CE2	TYR	A	196	21.376	-2.822	13.479	1.00	45.64	C
ATOM	1443	CD2	TYR	A	196	21.456	-4.129	13.910	1.00	46.66	C
ATOM	1444	C	TYR	A	196	21.447	-8.824	13.301	1.00	51.26	C
ATOM	1445	O	TYR	A	196	20.619	-9.391	14.003	1.00	51.19	O
ATOM	1446	N	GLU	A	197	22.539	-9.402	12.852	1.00	51.92	N
ATOM	1447	CA	GLU	A	197	22.729	-10.835	12.988	1.00	53.08	C
ATOM	1448	CB	GLU	A	197	23.664	-11.336	11.873	1.00	53.73	C
ATOM	1449	CG	GLU	A	197	23.493	-10.569	10.549	1.00	55.31	C
ATOM	1450	CD	GLU	A	197	24.587	-10.859	9.515	1.00	58.33	C
ATOM	1451	OE1	GLU	A	197	25.303	-11.910	9.660	1.00	58.85	O
ATOM	1452	OE2	GLU	A	197	24.721	-10.030	8.558	1.00	57.96	O
ATOM	1453	C	GLU	A	197	23.156	-11.288	14.402	1.00	52.92	C

227/396

Figure 3A-27

ATOM	1454	O	GLU	A	197	23.134	-12.497	14.708	1.00	53.24	O
ATOM	1455	N	ASP	A	198	23.542	-10.307	15.227	1.00	52.53	N
ATOM	1456	CA	ASP	A	198	23.778	-10.424	16.679	1.00	52.89	C
ATOM	1457	CB	ASP	A	198	24.600	-11.655	17.069	1.00	53.46	C
ATOM	1458	CG	ASP	A	198	25.760	-11.933	16.122	1.00	56.20	C
ATOM	1459	OD1	ASP	A	198	25.756	-13.058	15.518	1.00	58.36	O
ATOM	1460	OD2	ASP	A	198	26.713	-11.115	15.945	1.00	57.80	O
ATOM	1461	C	ASP	A	198	24.505	-9.180	17.133	1.00	52.34	C
ATOM	1462	O	ASP	A	198	25.297	-8.671	16.370	1.00	53.02	O
ATOM	1463	N	TYR	A	199	24.262	-8.682	18.344	1.00	51.32	N
ATOM	1464	CA	TYR	A	199	24.889	-7.428	18.784	1.00	50.83	C
ATOM	1465	CB	TYR	A	199	25.052	-7.382	20.308	1.00	50.83	C
ATOM	1466	CG	TYR	A	199	25.309	-5.998	20.900	1.00	51.82	C
ATOM	1467	CD1	TYR	A	199	24.550	-4.877	20.520	1.00	53.73	C
ATOM	1468	CE1	TYR	A	199	24.778	-3.598	21.069	1.00	54.77	C
ATOM	1469	CZ	TYR	A	199	25.776	-3.434	22.011	1.00	56.22	C
ATOM	1470	OH	TYR	A	199	26.023	-2.192	22.570	1.00	56.97	O
ATOM	1471	CE2	TYR	A	199	26.529	-4.535	22.417	1.00	55.69	C
ATOM	1472	CD2	TYR	A	199	26.291	-5.812	21.856	1.00	53.61	C
ATOM	1473	C	TYR	A	199	26.230	-7.097	18.109	1.00	50.59	C
ATOM	1474	O	TYR	A	199	26.501	-5.944	17.820	1.00	50.81	O
ATOM	1475	N	GLY	A	200	27.073	-8.099	17.867	1.00	50.29	N
ATOM	1476	CA	GLY	A	200	28.327	-7.907	17.145	1.00	49.72	C
ATOM	1477	C	GLY	A	200	28.050	-7.256	15.809	1.00	49.51	C
ATOM	1478	O	GLY	A	200	28.470	-6.127	15.563	1.00	49.34	O
ATOM	1479	N	ASP	A	201	27.307	-7.963	14.956	1.00	49.33	N
ATOM	1480	CA	ASP	A	201	26.852	-7.405	13.685	1.00	48.60	C
ATOM	1481	CB	ASP	A	201	25.716	-8.246	13.054	1.00	48.82	C
ATOM	1482	CG	ASP	A	201	25.263	-7.726	11.654	1.00	50.77	C
ATOM	1483	OD1	ASP	A	201	26.069	-7.667	10.690	1.00	51.63	O
ATOM	1484	OD2	ASP	A	201	24.085	-7.371	11.412	1.00	52.97	O
ATOM	1485	C	ASP	A	201	26.485	-5.948	13.935	1.00	47.61	C
ATOM	1486	O	ASP	A	201	26.858	-5.099	13.148	1.00	47.76	O
ATOM	1487	N	TYR	A	202	25.844	-5.649	15.061	1.00	46.27	N
ATOM	1488	CA	TYR	A	202	25.537	-4.264	15.385	1.00	45.79	C
ATOM	1489	CB	TYR	A	202	24.600	-4.188	16.602	1.00	46.41	C
ATOM	1490	CG	TYR	A	202	24.151	-2.803	17.092	1.00	47.29	C
ATOM	1491	CD1	TYR	A	202	23.164	-2.082	16.427	1.00	47.77	C
ATOM	1492	CE1	TYR	A	202	22.731	-0.838	16.884	1.00	48.40	C
ATOM	1493	CZ	TYR	A	202	23.277	-0.306	18.029	1.00	50.75	C
ATOM	1494	OH	TYR	A	202	22.849	0.927	18.499	1.00	51.51	O
ATOM	1495	CE2	TYR	A	202	24.254	-1.017	18.731	1.00	51.26	C
ATOM	1496	CD2	TYR	A	202	24.673	-2.258	18.263	1.00	49.02	C
ATOM	1497	C	TYR	A	202	26.808	-3.384	15.505	1.00	45.18	C
ATOM	1498	O	TYR	A	202	27.068	-2.589	14.618	1.00	45.51	O
ATOM	1499	N	TRP	A	203	27.636	-3.520	16.540	1.00	44.27	N
ATOM	1500	CA	TRP	A	203	28.764	-2.561	16.713	1.00	43.20	C
ATOM	1501	CB	TRP	A	203	29.791	-3.031	17.766	1.00	43.88	C
ATOM	1502	CG	TRP	A	203	29.406	-2.773	19.199	1.00	45.24	C
ATOM	1503	CD1	TRP	A	203	28.616	-1.756	19.678	1.00	47.70	C
ATOM	1504	NE1	TRP	A	203	28.473	-1.863	21.041	1.00	48.16	N
ATOM	1505	CE2	TRP	A	203	29.192	-2.946	21.473	1.00	47.59	C
ATOM	1506	CD2	TRP	A	203	29.793	-3.541	20.333	1.00	45.51	C
ATOM	1507	CE3	TRP	A	203	30.587	-4.672	20.510	1.00	45.22	C
ATOM	1508	CZ3	TRP	A	203	30.772	-5.169	21.795	1.00	47.24	C
ATOM	1509	CH2	TRP	A	203	30.166	-4.557	22.915	1.00	48.83	C

228/396

Figure 3A-28

ATOM	1510	CZ2	TRP	A	203	29.374	-3.444	22.775	1.00	48.67	C
ATOM	1511	C	TRP	A	203	29.489	-2.322	15.403	1.00	41.71	C
ATOM	1512	O	TRP	A	203	30.254	-1.378	15.267	1.00	41.50	O
ATOM	1513	N	ARG	A	204	29.243	-3.218	14.458	1.00	40.02	N
ATOM	1514	CA	ARG	A	204	29.957	-3.248	13.221	1.00	38.87	C
ATOM	1515	CB	ARG	A	204	29.801	-4.604	12.557	1.00	38.57	C
ATOM	1516	CG	ARG	A	204	30.606	-5.742	13.184	1.00	37.80	C
ATOM	1517	CD	ARG	A	204	31.173	-6.766	12.183	1.00	34.82	C
ATOM	1518	NE	ARG	A	204	30.351	-7.967	12.010	1.00	29.47	N
ATOM	1519	CZ	ARG	A	204	29.985	-8.762	13.000	1.00	29.29	C
ATOM	1520	NH1	ARG	A	204	30.333	-8.497	14.258	1.00	28.02	N
ATOM	1521	NH2	ARG	A	204	29.253	-9.831	12.741	1.00	30.87	N
ATOM	1522	C	ARG	A	204	29.246	-2.262	12.408	1.00	38.59	C
ATOM	1523	O	ARG	A	204	29.810	-1.685	11.496	1.00	39.09	O
ATOM	1524	N	GLY	A	205	27.990	-2.057	12.756	1.00	38.21	N
ATOM	1525	CA	GLY	A	205	27.086	-1.287	11.940	1.00	38.40	C
ATOM	1526	C	GLY	A	205	27.837	-0.060	11.578	1.00	38.73	C
ATOM	1527	O	GLY	A	205	27.949	0.299	10.410	1.00	38.98	O
ATOM	1528	N	ASP	A	206	28.437	0.530	12.595	1.00	39.25	N
ATOM	1529	CA	ASP	A	206	29.183	1.773	12.450	1.00	40.02	C
ATOM	1530	CB	ASP	A	206	30.062	2.020	13.649	1.00	39.57	C
ATOM	1531	CG	ASP	A	206	30.287	3.448	13.853	1.00	39.91	C
ATOM	1532	OD1	ASP	A	206	31.227	3.987	13.243	1.00	40.49	O
ATOM	1533	OD2	ASP	A	206	29.518	4.136	14.543	1.00	42.90	O
ATOM	1534	C	ASP	A	206	30.037	1.944	11.221	1.00	40.92	C
ATOM	1535	O	ASP	A	206	30.405	3.061	10.899	1.00	41.10	O
ATOM	1536	N	TYR	A	207	30.360	0.859	10.533	1.00	42.44	N
ATOM	1537	CA	TYR	A	207	31.265	0.976	9.413	1.00	43.87	C
ATOM	1538	CB	TYR	A	207	32.342	-0.074	9.498	1.00	43.31	C
ATOM	1539	CG	TYR	A	207	33.328	0.338	10.552	1.00	42.02	C
ATOM	1540	CD1	TYR	A	207	33.224	-0.159	11.845	1.00	41.53	C
ATOM	1541	CE1	TYR	A	207	34.095	0.220	12.836	1.00	40.22	C
ATOM	1542	CZ	TYR	A	207	35.071	1.121	12.539	1.00	40.23	C
ATOM	1543	OH	TYR	A	207	35.922	1.485	13.539	1.00	39.58	O
ATOM	1544	CE2	TYR	A	207	35.197	1.646	11.254	1.00	40.65	C
ATOM	1545	CD2	TYR	A	207	34.314	1.273	10.282	1.00	40.33	C
ATOM	1546	C	TYR	A	207	30.590	1.041	8.070	1.00	45.64	C
ATOM	1547	O	TYR	A	207	31.227	1.395	7.063	1.00	45.78	O
ATOM	1548	N	GLU	A	208	29.286	0.749	8.095	1.00	47.67	N
ATOM	1549	CA	GLU	A	208	28.406	0.681	6.907	1.00	49.56	C
ATOM	1550	CB	GLU	A	208	27.063	0.108	7.329	1.00	49.30	C
ATOM	1551	CG	GLU	A	208	26.272	-0.587	6.247	1.00	50.36	C
ATOM	1552	CD	GLU	A	208	25.250	-1.545	6.851	1.00	53.52	C
ATOM	1553	OE1	GLU	A	208	24.979	-1.451	8.083	1.00	54.11	O
ATOM	1554	OE2	GLU	A	208	24.713	-2.405	6.108	1.00	55.31	O
ATOM	1555	C	GLU	A	208	28.144	1.990	6.129	1.00	50.45	C
ATOM	1556	O	GLU	A	208	27.804	3.016	6.714	1.00	50.52	O
ATOM	1557	N	VAL	A	209	28.304	1.950	4.811	1.00	51.55	N
ATOM	1558	CA	VAL	A	209	27.677	2.962	3.976	1.00	53.16	C
ATOM	1559	CB	VAL	A	209	28.596	4.210	3.595	1.00	52.85	C
ATOM	1560	CG1	VAL	A	209	29.490	4.626	4.753	1.00	53.20	C
ATOM	1561	CG2	VAL	A	209	29.406	3.992	2.345	1.00	52.23	C
ATOM	1562	C	VAL	A	209	26.936	2.270	2.807	1.00	54.65	C
ATOM	1563	O	VAL	A	209	27.532	1.475	2.068	1.00	54.81	O
ATOM	1564	N	ASN	A	210	25.620	2.546	2.716	1.00	56.22	N
ATOM	1565	CA	ASN	A	210	24.699	1.988	1.716	1.00	57.15	C

229/396

Figure 3A-29

ATOM	1566	CB	ASN	A	210	23.372	1.545	2.366	1.00	57.00	C
ATOM	1567	CG	ASN	A	210	23.513	0.302	3.277	1.00	57.57	C
ATOM	1568	OD1	ASN	A	210	23.353	0.395	4.509	1.00	57.56	O
ATOM	1569	ND2	ASN	A	210	23.764	-0.866	2.669	1.00	57.38	N
ATOM	1570	C	ASN	A	210	24.425	3.027	0.620	1.00	57.95	C
ATOM	1571	O	ASN	A	210	24.915	2.898	-0.513	1.00	57.90	O
ATOM	1572	N	GLY	A	211	23.661	4.059	0.987	1.00	58.83	N
ATOM	1573	CA	GLY	A	211	23.270	5.146	0.100	1.00	60.03	C
ATOM	1574	C	GLY	A	211	24.142	5.480	-1.118	1.00	60.82	C
ATOM	1575	O	GLY	A	211	23.610	5.795	-2.198	1.00	61.11	O
ATOM	1576	N	VAL	A	212	25.471	5.430	-0.975	1.00	61.00	N
ATOM	1577	CA	VAL	A	212	26.332	5.835	-2.095	1.00	60.85	C
ATOM	1578	CB	VAL	A	212	27.385	6.908	-1.703	1.00	60.69	C
ATOM	1579	CG1	VAL	A	212	27.872	7.618	-2.940	1.00	60.80	C
ATOM	1580	CG2	VAL	A	212	26.819	7.931	-0.706	1.00	59.97	C
ATOM	1581	C	VAL	A	212	26.967	4.668	-2.877	1.00	61.06	C
ATOM	1582	O	VAL	A	212	27.331	3.630	-2.316	1.00	61.06	O
ATOM	1583	N	ASP	A	213	27.048	4.857	-4.187	1.00	61.28	N
ATOM	1584	CA	ASP	A	213	27.703	3.922	-5.072	1.00	61.70	C
ATOM	1585	CB	ASP	A	213	27.048	3.943	-6.444	1.00	62.18	C
ATOM	1586	CG	ASP	A	213	26.740	2.551	-6.947	1.00	64.36	C
ATOM	1587	OD1	ASP	A	213	26.034	1.808	-6.203	1.00	65.62	O
ATOM	1588	OD2	ASP	A	213	27.166	2.119	-8.057	1.00	65.83	O
ATOM	1589	C	ASP	A	213	29.171	4.281	-5.211	1.00	61.43	C
ATOM	1590	O	ASP	A	213	29.539	5.464	-5.147	1.00	61.73	O
ATOM	1591	N	GLY	A	214	29.998	3.256	-5.427	1.00	60.79	N
ATOM	1592	CA	GLY	A	214	31.447	3.387	-5.378	1.00	59.77	C
ATOM	1593	C	GLY	A	214	31.927	3.243	-3.941	1.00	59.18	C
ATOM	1594	O	GLY	A	214	32.979	2.621	-3.681	1.00	59.22	O
ATOM	1595	N	TYR	A	215	31.107	3.780	-3.022	1.00	57.94	N
ATOM	1596	CA	TYR	A	215	31.445	4.022	-1.622	1.00	56.58	C
ATOM	1597	CB	TYR	A	215	31.042	5.435	-1.260	1.00	55.47	C
ATOM	1598	CG	TYR	A	215	31.766	6.433	-2.090	1.00	54.43	C
ATOM	1599	CD1	TYR	A	215	32.627	6.028	-3.114	1.00	53.94	C
ATOM	1600	CE1	TYR	A	215	33.324	6.940	-3.880	1.00	53.25	C
ATOM	1601	CZ	TYR	A	215	33.158	8.281	-3.630	1.00	52.78	C
ATOM	1602	OH	TYR	A	215	33.826	9.200	-4.371	1.00	52.85	O
ATOM	1603	CE2	TYR	A	215	32.313	8.715	-2.637	1.00	53.25	C
ATOM	1604	CD2	TYR	A	215	31.623	7.786	-1.861	1.00	54.42	C
ATOM	1605	C	TYR	A	215	30.791	3.047	-0.673	1.00	56.74	C
ATOM	1606	O	TYR	A	215	31.148	2.964	0.500	1.00	56.69	O
ATOM	1607	N	ASP	A	216	29.821	2.314	-1.186	1.00	56.83	N
ATOM	1608	CA	ASP	A	216	29.119	1.320	-0.414	1.00	57.21	C
ATOM	1609	CB	ASP	A	216	28.251	0.538	-1.399	1.00	57.77	C
ATOM	1610	CG	ASP	A	216	27.390	-0.518	-0.743	1.00	60.02	C
ATOM	1611	OD1	ASP	A	216	27.795	-1.726	-0.743	1.00	62.64	O
ATOM	1612	OD2	ASP	A	216	26.271	-0.231	-0.252	1.00	61.59	O
ATOM	1613	C	ASP	A	216	30.140	0.424	0.318	1.00	56.94	C
ATOM	1614	O	ASP	A	216	30.984	-0.216	-0.333	1.00	57.43	O
ATOM	1615	N	TYR	A	217	30.089	0.421	1.662	1.00	56.53	N
ATOM	1616	CA	TYR	A	217	30.904	-0.482	2.546	1.00	55.80	C
ATOM	1617	CB	TYR	A	217	31.935	0.319	3.383	1.00	55.32	C
ATOM	1618	CG	TYR	A	217	32.967	-0.546	4.058	1.00	52.12	C
ATOM	1619	CD1	TYR	A	217	34.191	-0.797	3.451	1.00	48.81	C
ATOM	1620	CE1	TYR	A	217	35.125	-1.610	4.054	1.00	48.71	C
ATOM	1621	CZ	TYR	A	217	34.838	-2.194	5.289	1.00	49.23	C

230/396

Figure 3A-30

ATOM	1622	OH	TYR	A	217	35.767	-2.989	5.917	1.00	48.40	O
ATOM	1623	CE2	TYR	A	217	33.630	-1.957	5.905	1.00	49.85	C
ATOM	1624	CD2	TYR	A	217	32.704	-1.127	5.290	1.00	50.90	C
ATOM	1625	C	TYR	A	217	30.059	-1.354	3.504	1.00	55.96	C
ATOM	1626	O	TYR	A	217	29.367	-0.826	4.389	1.00	56.09	O
ATOM	1627	N	SER	A	218	30.111	-2.674	3.363	1.00	55.67	N
ATOM	1628	CA	SER	A	218	29.154	-3.469	4.140	1.00	55.89	C
ATOM	1629	CB	SER	A	218	28.631	-4.694	3.364	1.00	56.21	C
ATOM	1630	OG	SER	A	218	29.671	-5.478	2.793	1.00	56.91	O
ATOM	1631	C	SER	A	218	29.648	-3.859	5.521	1.00	55.51	C
ATOM	1632	O	SER	A	218	30.813	-3.697	5.841	1.00	55.70	O
ATOM	1633	N	ARG	A	219	28.748	-4.371	6.339	1.00	55.23	N
ATOM	1634	CA	ARG	A	219	29.139	-4.854	7.636	1.00	55.41	C
ATOM	1635	CB	ARG	A	219	27.920	-5.285	8.420	1.00	55.75	C
ATOM	1636	CG	ARG	A	219	27.804	-4.617	9.771	1.00	57.76	C
ATOM	1637	CD	ARG	A	219	26.549	-4.988	10.495	1.00	62.05	C
ATOM	1638	NE	ARG	A	219	25.513	-5.313	9.523	1.00	67.22	N
ATOM	1639	CZ	ARG	A	219	24.664	-4.416	9.014	1.00	70.31	C
ATOM	1640	NH1	ARG	A	219	24.702	-3.137	9.424	1.00	70.59	N
ATOM	1641	NH2	ARG	A	219	23.767	-4.800	8.104	1.00	70.76	N
ATOM	1642	C	ARG	A	219	30.068	-6.032	7.472	1.00	55.22	C
ATOM	1643	O	ARG	A	219	31.110	-6.103	8.120	1.00	54.95	O
ATOM	1644	N	GLY	A	220	29.685	-6.960	6.596	1.00	55.35	N
ATOM	1645	CA	GLY	A	220	30.488	-8.147	6.345	1.00	54.91	C
ATOM	1646	C	GLY	A	220	31.945	-7.772	6.189	1.00	54.26	C
ATOM	1647	O	GLY	A	220	32.817	-8.326	6.866	1.00	53.62	O
ATOM	1648	N	GLN	A	221	32.160	-6.778	5.326	1.00	54.05	N
ATOM	1649	CA	GLN	A	221	33.465	-6.329	4.888	1.00	54.05	C
ATOM	1650	CB	GLN	A	221	33.365	-5.128	3.989	1.00	54.15	C
ATOM	1651	CG	GLN	A	221	34.461	-5.137	2.964	1.00	57.26	C
ATOM	1652	CD	GLN	A	221	33.945	-5.443	1.564	1.00	62.06	C
ATOM	1653	OE1	GLN	A	221	33.068	-4.721	1.046	1.00	64.80	O
ATOM	1654	NE2	GLN	A	221	34.474	-6.506	0.944	1.00	62.96	N
ATOM	1655	C	GLN	A	221	34.357	-5.968	6.016	1.00	53.80	C
ATOM	1656	O	GLN	A	221	35.428	-6.560	6.148	1.00	54.23	O
ATOM	1657	N	LEU	A	222	33.932	-4.984	6.815	1.00	53.22	N
ATOM	1658	CA	LEU	A	222	34.617	-4.603	8.077	1.00	52.25	C
ATOM	1659	CB	LEU	A	222	33.623	-3.939	9.026	1.00	52.04	C
ATOM	1660	CG	LEU	A	222	34.010	-3.319	10.367	1.00	51.60	C
ATOM	1661	CD1	LEU	A	222	33.915	-4.398	11.470	1.00	50.88	C
ATOM	1662	CD2	LEU	A	222	35.353	-2.530	10.359	1.00	49.47	C
ATOM	1663	C	LEU	A	222	35.440	-5.707	8.802	1.00	51.57	C
ATOM	1664	O	LEU	A	222	36.515	-5.420	9.307	1.00	50.88	O
ATOM	1665	N	ILE	A	223	34.952	-6.952	8.845	1.00	51.16	N
ATOM	1666	CA	ILE	A	223	35.827	-8.047	9.241	1.00	50.78	C
ATOM	1667	CB	ILE	A	223	35.121	-9.391	9.399	1.00	50.37	C
ATOM	1668	CG1	ILE	A	223	34.218	-9.414	10.624	1.00	48.92	C
ATOM	1669	CD1	ILE	A	223	33.465	-10.732	10.787	1.00	48.18	C
ATOM	1670	CG2	ILE	A	223	36.170	-10.490	9.529	1.00	49.11	C
ATOM	1671	C	ILE	A	223	36.848	-8.189	8.156	1.00	51.38	C
ATOM	1672	O	ILE	A	223	38.001	-7.850	8.349	1.00	51.57	O
ATOM	1673	N	GLU	A	224	36.400	-8.662	7.000	1.00	52.27	N
ATOM	1674	CA	GLU	A	224	37.299	-9.042	5.910	1.00	53.43	C
ATOM	1675	CB	GLU	A	224	36.524	-9.458	4.610	1.00	54.21	C
ATOM	1676	CG	GLU	A	224	35.907	-8.352	3.720	1.00	56.58	C
ATOM	1677	CD	GLU	A	224	36.541	-8.227	2.320	1.00	58.73	C

231/396

Figure 3A-31

ATOM	1678	OE1	GLU	A	224	36.923	-9.284	1.750	1.00	60.36	O
ATOM	1679	OE2	GLU	A	224	36.666	-7.079	1.788	1.00	56.57	O
ATOM	1680	C	GLU	A	224	38.425	-8.023	5.685	1.00	53.05	C
ATOM	1681	O	GLU	A	224	39.542	-8.385	5.372	1.00	52.61	O
ATOM	1682	N	ASP	A	225	38.141	-6.755	5.907	1.00	53.36	N
ATOM	1683	CA	ASP	A	225	39.186	-5.748	5.812	1.00	54.14	C
ATOM	1684	CB	ASP	A	225	38.585	-4.429	5.345	1.00	54.31	C
ATOM	1685	CG	ASP	A	225	38.013	-4.539	3.971	1.00	55.23	C
ATOM	1686	OD1	ASP	A	225	37.944	-5.680	3.461	1.00	54.90	O
ATOM	1687	OD2	ASP	A	225	37.621	-3.549	3.317	1.00	58.05	O
ATOM	1688	C	ASP	A	225	40.009	-5.561	7.099	1.00	54.21	C
ATOM	1689	O	ASP	A	225	40.990	-4.816	7.126	1.00	54.48	O
ATOM	1690	N	VAL	A	226	39.606	-6.214	8.171	1.00	53.72	N
ATOM	1691	CA	VAL	A	226	40.387	-6.127	9.357	1.00	53.40	C
ATOM	1692	CB	VAL	A	226	39.511	-5.901	10.600	1.00	53.64	C
ATOM	1693	CG1	VAL	A	226	40.014	-6.622	11.839	1.00	53.73	C
ATOM	1694	CG2	VAL	A	226	39.434	-4.406	10.876	1.00	54.19	C
ATOM	1695	C	VAL	A	226	41.146	-7.395	9.296	1.00	53.31	C
ATOM	1696	O	VAL	A	226	42.287	-7.419	9.687	1.00	54.02	O
ATOM	1697	N	GLU	A	227	40.538	-8.427	8.723	1.00	53.26	N
ATOM	1698	CA	GLU	A	227	41.223	-9.696	8.448	1.00	53.49	C
ATOM	1699	CB	GLU	A	227	40.366	-10.610	7.550	1.00	53.81	C
ATOM	1700	CG	GLU	A	227	39.106	-11.181	8.172	1.00	56.08	C
ATOM	1701	CD	GLU	A	227	39.394	-11.924	9.461	1.00	59.84	C
ATOM	1702	OE1	GLU	A	227	38.455	-12.583	10.000	1.00	60.34	O
ATOM	1703	OE2	GLU	A	227	40.568	-11.841	9.922	1.00	60.68	O
ATOM	1704	C	GLU	A	227	42.576	-9.506	7.753	1.00	52.98	C
ATOM	1705	O	GLU	A	227	43.636	-9.652	8.373	1.00	53.30	O
ATOM	1706	N	HIS	A	228	42.526	-9.162	6.469	1.00	51.80	N
ATOM	1707	CA	HIS	A	228	43.688	-9.213	5.602	1.00	51.08	C
ATOM	1708	CB	HIS	A	228	43.209	-9.257	4.133	1.00	51.44	C
ATOM	1709	CG	HIS	A	228	43.959	-8.389	3.161	1.00	52.26	C
ATOM	1710	ND1	HIS	A	228	43.955	-7.008	3.218	1.00	52.81	N
ATOM	1711	CE1	HIS	A	228	44.646	-6.525	2.200	1.00	53.11	C
ATOM	1712	NE2	HIS	A	228	45.073	-7.539	1.467	1.00	52.97	N
ATOM	1713	CD2	HIS	A	228	44.643	-8.714	2.035	1.00	52.50	C
ATOM	1714	C	HIS	A	228	44.720	-8.142	5.956	1.00	50.51	C
ATOM	1715	O	HIS	A	228	45.908	-8.432	6.132	1.00	51.07	O
ATOM	1716	N	THR	A	229	44.266	-6.915	6.128	1.00	49.44	N
ATOM	1717	CA	THR	A	229	45.134	-5.870	6.634	1.00	48.08	C
ATOM	1718	CB	THR	A	229	44.328	-4.604	6.868	1.00	47.94	C
ATOM	1719	OG1	THR	A	229	45.228	-3.520	7.029	1.00	48.85	O
ATOM	1720	CG2	THR	A	229	43.583	-4.630	8.189	1.00	46.89	C
ATOM	1721	C	THR	A	229	45.884	-6.286	7.894	1.00	47.54	C
ATOM	1722	O	THR	A	229	46.967	-5.805	8.136	1.00	47.01	O
ATOM	1723	N	PHE	A	230	45.313	-7.180	8.691	1.00	47.55	N
ATOM	1724	CA	PHE	A	230	46.037	-7.722	9.822	1.00	48.57	C
ATOM	1725	CB	PHE	A	230	45.204	-8.736	10.598	1.00	48.62	C
ATOM	1726	CG	PHE	A	230	45.823	-9.169	11.916	1.00	48.70	C
ATOM	1727	CD1	PHE	A	230	47.107	-8.811	12.260	1.00	47.93	C
ATOM	1728	CE1	PHE	A	230	47.646	-9.198	13.471	1.00	48.84	C
ATOM	1729	CZ	PHE	A	230	46.917	-9.961	14.349	1.00	48.74	C
ATOM	1730	CE2	PHE	A	230	45.640	-10.327	14.032	1.00	49.06	C
ATOM	1731	CD2	PHE	A	230	45.095	-9.936	12.815	1.00	49.90	C
ATOM	1732	C	PHE	A	230	47.243	-8.424	9.256	1.00	49.42	C
ATOM	1733	O	PHE	A	230	48.239	-7.785	8.933	1.00	49.52	O

232/396

Figure 3A-32

ATOM	1734	N	GLU	A	231	47.140	-9.751	9.173	1.00	50.25	N
ATOM	1735	CA	GLU	A	231	47.932	-10.584	8.266	1.00	50.65	C
ATOM	1736	CB	GLU	A	231	47.032	-11.182	7.182	1.00	50.51	C
ATOM	1737	CG	GLU	A	231	46.916	-12.673	7.308	1.00	53.86	C
ATOM	1738	CD	GLU	A	231	48.276	-13.340	7.564	1.00	60.28	C
ATOM	1739	OE1	GLU	A	231	49.190	-13.262	6.673	1.00	62.10	O
ATOM	1740	OE2	GLU	A	231	48.434	-13.953	8.660	1.00	60.78	O
ATOM	1741	C	GLU	A	231	49.182	-9.953	7.633	1.00	50.21	C
ATOM	1742	O	GLU	A	231	50.170	-10.669	7.450	1.00	50.48	O
ATOM	1743	N	GLU	A	232	49.134	-8.653	7.286	1.00	49.36	N
ATOM	1744	CA	GLU	A	232	50.333	-7.898	6.896	1.00	48.83	C
ATOM	1745	CB	GLU	A	232	50.018	-6.763	5.917	1.00	48.82	C
ATOM	1746	CG	GLU	A	232	48.787	-6.935	5.035	1.00	52.37	C
ATOM	1747	CD	GLU	A	232	49.020	-6.499	3.565	1.00	58.32	C
ATOM	1748	OE1	GLU	A	232	48.197	-6.902	2.688	1.00	58.68	O
ATOM	1749	OE2	GLU	A	232	50.024	-5.763	3.265	1.00	60.40	O
ATOM	1750	C	GLU	A	232	51.043	-7.299	8.106	1.00	48.09	C
ATOM	1751	O	GLU	A	232	51.937	-6.461	7.941	1.00	48.51	O
ATOM	1752	N	ILE	A	233	50.646	-7.690	9.318	1.00	46.91	N
ATOM	1753	CA	ILE	A	233	51.157	-7.009	10.506	1.00	45.58	C
ATOM	1754	CB	ILE	A	233	50.032	-6.335	11.311	1.00	45.41	C
ATOM	1755	CG1	ILE	A	233	49.795	-4.925	10.780	1.00	44.76	C
ATOM	1756	CD1	ILE	A	233	50.791	-3.930	11.307	1.00	45.40	C
ATOM	1757	CG2	ILE	A	233	50.344	-6.290	12.801	1.00	44.07	C
ATOM	1758	C	ILE	A	233	52.055	-7.867	11.361	1.00	45.28	C
ATOM	1759	O	ILE	A	233	53.141	-7.436	11.695	1.00	46.03	O
ATOM	1760	N	LYS	A	234	51.619	-9.079	11.689	1.00	44.24	N
ATOM	1761	CA	LYS	A	234	52.477	-10.118	12.283	1.00	43.25	C
ATOM	1762	CB	LYS	A	234	51.782	-11.483	12.133	1.00	43.35	C
ATOM	1763	CG	LYS	A	234	50.361	-11.377	11.572	1.00	44.06	C
ATOM	1764	CD	LYS	A	234	49.886	-12.648	10.869	1.00	45.75	C
ATOM	1765	CE	LYS	A	234	48.893	-13.482	11.748	1.00	46.30	C
ATOM	1766	NZ	LYS	A	234	48.612	-14.884	11.244	1.00	43.44	N
ATOM	1767	C	LYS	A	234	53.940	-10.168	11.735	1.00	42.44	C
ATOM	1768	O	LYS	A	234	54.886	-10.402	12.502	1.00	41.66	O
ATOM	1769	N	PRO	A	235	54.128	-9.960	10.422	1.00	41.91	N
ATOM	1770	CA	PRO	A	235	55.468	-9.723	9.852	1.00	41.54	C
ATOM	1771	CB	PRO	A	235	55.153	-9.084	8.491	1.00	41.58	C
ATOM	1772	CG	PRO	A	235	53.814	-9.646	8.098	1.00	41.64	C
ATOM	1773	CD	PRO	A	235	53.099	-10.004	9.361	1.00	41.76	C
ATOM	1774	C	PRO	A	235	56.391	-8.778	10.655	1.00	40.98	C
ATOM	1775	O	PRO	A	235	57.604	-8.747	10.390	1.00	41.16	O
ATOM	1776	N	LEU	A	236	55.815	-8.034	11.606	1.00	39.98	N
ATOM	1777	CA	LEU	A	236	56.480	-6.974	12.384	1.00	38.38	C
ATOM	1778	CB	LEU	A	236	56.212	-5.583	11.772	1.00	37.79	C
ATOM	1779	CG	LEU	A	236	56.165	-4.446	12.799	1.00	36.32	C
ATOM	1780	CD1	LEU	A	236	57.557	-3.910	12.970	1.00	34.81	C
ATOM	1781	CD2	LEU	A	236	55.166	-3.334	12.490	1.00	34.02	C
ATOM	1782	C	LEU	A	236	55.940	-6.998	13.812	1.00	37.83	C
ATOM	1783	O	LEU	A	236	56.512	-6.369	14.717	1.00	37.95	O
ATOM	1784	N	TYR	A	237	54.802	-7.666	14.013	1.00	36.99	N
ATOM	1785	CA	TYR	A	237	54.313	-7.833	15.367	1.00	36.01	C
ATOM	1786	CB	TYR	A	237	52.895	-8.413	15.453	1.00	34.47	C
ATOM	1787	CG	TYR	A	237	52.564	-8.864	16.863	1.00	30.46	C
ATOM	1788	CD1	TYR	A	237	52.820	-8.043	17.951	1.00	26.97	C
ATOM	1789	CE1	TYR	A	237	52.561	-8.473	19.243	1.00	25.17	C

233/396

Figure 3A-33

ATOM	1790	CZ	TYR	A	237	52.029	-9.727	19.451	1.00	24.62	C
ATOM	1791	OH	TYR	A	237	51.783	-10.140	20.725	1.00	24.89	O
ATOM	1792	CE2	TYR	A	237	51.742	-10.559	18.396	1.00	24.10	C
ATOM	1793	CD2	TYR	A	237	52.034	-10.133	17.112	1.00	27.63	C
ATOM	1794	C	TYR	A	237	55.358	-8.768	15.955	1.00	36.95	C
ATOM	1795	O	TYR	A	237	56.153	-8.368	16.844	1.00	37.11	O
ATOM	1796	N	GLU	A	238	55.380	-9.983	15.393	1.00	37.31	N
ATOM	1797	CA	GLU	A	238	56.412	-10.981	15.666	1.00	36.85	C
ATOM	1798	CB	GLU	A	238	56.409	-12.097	14.601	1.00	36.95	C
ATOM	1799	CG	GLU	A	238	55.168	-13.003	14.722	1.00	35.19	C
ATOM	1800	CD	GLU	A	238	54.962	-13.961	13.552	1.00	32.91	C
ATOM	1801	OE1	GLU	A	238	54.724	-15.162	13.808	1.00	31.05	O
ATOM	1802	OE2	GLU	A	238	55.019	-13.511	12.385	1.00	31.95	O
ATOM	1803	C	GLU	A	238	57.779	-10.330	15.924	1.00	36.53	C
ATOM	1804	O	GLU	A	238	58.108	-10.132	17.077	1.00	36.60	O
ATOM	1805	N	HIS	A	239	58.549	-9.924	14.928	1.00	35.94	N
ATOM	1806	CA	HIS	A	239	59.847	-9.345	15.302	1.00	36.40	C
ATOM	1807	CB	HIS	A	239	60.528	-8.600	14.157	1.00	37.46	C
ATOM	1808	CG	HIS	A	239	61.257	-9.507	13.196	1.00	42.14	C
ATOM	1809	ND1	HIS	A	239	62.635	-9.593	13.141	1.00	44.33	N
ATOM	1810	CE1	HIS	A	239	62.979	-10.462	12.206	1.00	46.08	C
ATOM	1811	NE2	HIS	A	239	61.881	-10.949	11.654	1.00	46.44	N
ATOM	1812	CD2	HIS	A	239	60.790	-10.369	12.253	1.00	45.60	C
ATOM	1813	C	HIS	A	239	59.828	-8.551	16.625	1.00	35.28	C
ATOM	1814	O	HIS	A	239	60.413	-8.980	17.601	1.00	35.42	O
ATOM	1815	N	LEU	A	240	59.118	-7.446	16.695	1.00	34.63	N
ATOM	1816	CA	LEU	A	240	58.923	-6.751	17.966	1.00	34.50	C
ATOM	1817	CB	LEU	A	240	57.822	-5.719	17.788	1.00	34.72	C
ATOM	1818	CG	LEU	A	240	57.604	-4.507	18.725	1.00	36.17	C
ATOM	1819	CD1	LEU	A	240	56.892	-4.987	19.982	1.00	38.25	C
ATOM	1820	CD2	LEU	A	240	58.809	-3.551	19.064	1.00	33.18	C
ATOM	1821	C	LEU	A	240	58.595	-7.662	19.169	1.00	34.37	C
ATOM	1822	O	LEU	A	240	59.005	-7.388	20.298	1.00	33.68	O
ATOM	1823	N	HIS	A	241	57.851	-8.741	18.924	1.00	34.71	N
ATOM	1824	CA	HIS	A	241	57.444	-9.695	19.973	1.00	34.83	C
ATOM	1825	CB	HIS	A	241	56.466	-10.725	19.425	1.00	34.56	C
ATOM	1826	CG	HIS	A	241	56.154	-11.844	20.378	1.00	35.03	C
ATOM	1827	ND1	HIS	A	241	56.445	-13.161	20.103	1.00	35.13	N
ATOM	1828	CE1	HIS	A	241	56.004	-13.925	21.089	1.00	35.53	C
ATOM	1829	NE2	HIS	A	241	55.440	-13.152	21.998	1.00	35.01	N
ATOM	1830	CD2	HIS	A	241	55.521	-11.846	21.577	1.00	35.64	C
ATOM	1831	C	HIS	A	241	58.609	-10.474	20.433	1.00	35.20	C
ATOM	1832	O	HIS	A	241	58.860	-10.533	21.628	1.00	35.17	O
ATOM	1833	N	ALA	A	242	59.252	-11.120	19.444	1.00	35.66	N
ATOM	1834	CA	ALA	A	242	60.451	-11.933	19.583	1.00	35.85	C
ATOM	1835	CB	ALA	A	242	60.886	-12.449	18.264	1.00	34.95	C
ATOM	1836	C	ALA	A	242	61.548	-11.103	20.215	1.00	36.58	C
ATOM	1837	O	ALA	A	242	62.065	-11.490	21.291	1.00	37.01	O
ATOM	1838	N	TYR	A	243	61.870	-9.951	19.604	1.00	36.99	N
ATOM	1839	CA	TYR	A	243	62.847	-9.017	20.214	1.00	37.83	C
ATOM	1840	CB	TYR	A	243	63.110	-7.748	19.392	1.00	37.19	C
ATOM	1841	CG	TYR	A	243	63.844	-6.577	20.095	1.00	34.78	C
ATOM	1842	CD1	TYR	A	243	64.853	-5.886	19.437	1.00	35.01	C
ATOM	1843	CE1	TYR	A	243	65.512	-4.814	20.019	1.00	33.62	C
ATOM	1844	CZ	TYR	A	243	65.169	-4.398	21.276	1.00	33.55	C
ATOM	1845	OH	TYR	A	243	65.823	-3.287	21.804	1.00	34.08	O

234/396

Figure 3A-34

ATOM	1846	CE2	TYR	A	243	64.166	-5.068	21.962	1.00	32.19	C
ATOM	1847	CD2	TYR	A	243	63.500	-6.134	21.360	1.00	31.33	C
ATOM	1848	C	TYR	A	243	62.486	-8.584	21.621	1.00	38.95	C
ATOM	1849	O	TYR	A	243	63.304	-7.965	22.278	1.00	39.68	O
ATOM	1850	N	VAL	A	244	61.288	-8.850	22.104	1.00	39.80	N
ATOM	1851	CA	VAL	A	244	61.109	-8.479	23.483	1.00	40.69	C
ATOM	1852	CB	VAL	A	244	59.829	-7.583	23.827	1.00	41.21	C
ATOM	1853	CG1	VAL	A	244	59.899	-6.215	23.100	1.00	40.60	C
ATOM	1854	CG2	VAL	A	244	58.475	-8.317	23.597	1.00	41.71	C
ATOM	1855	C	VAL	A	244	61.336	-9.650	24.368	1.00	40.97	C
ATOM	1856	O	VAL	A	244	61.993	-9.485	25.381	1.00	40.99	O
ATOM	1857	N	ARG	A	245	60.855	-10.840	23.973	1.00	41.60	N
ATOM	1858	CA	ARG	A	245	60.983	-12.015	24.848	1.00	42.33	C
ATOM	1859	CB	ARG	A	245	60.520	-13.343	24.227	1.00	41.69	C
ATOM	1860	CG	ARG	A	245	60.911	-13.573	22.772	1.00	42.71	C
ATOM	1861	CD	ARG	A	245	60.411	-14.909	22.167	1.00	43.90	C
ATOM	1862	NE	ARG	A	245	59.662	-15.707	23.157	1.00	43.98	N
ATOM	1863	CZ	ARG	A	245	58.765	-16.662	22.872	1.00	42.96	C
ATOM	1864	NH1	ARG	A	245	58.150	-17.287	23.856	1.00	40.67	N
ATOM	1865	NH2	ARG	A	245	58.477	-16.991	21.614	1.00	43.23	N
ATOM	1866	C	ARG	A	245	62.446	-12.037	25.242	1.00	43.10	C
ATOM	1867	O	ARG	A	245	62.790	-12.383	26.382	1.00	43.34	O
ATOM	1868	N	ALA	A	246	63.283	-11.600	24.294	1.00	43.31	N
ATOM	1869	CA	ALA	A	246	64.626	-11.126	24.582	1.00	43.19	C
ATOM	1870	CB	ALA	A	246	65.203	-10.491	23.346	1.00	43.53	C
ATOM	1871	C	ALA	A	246	64.633	-10.130	25.757	1.00	43.13	C
ATOM	1872	O	ALA	A	246	64.419	-10.525	26.889	1.00	42.75	O
ATOM	1873	N	LYS	A	247	64.831	-8.843	25.488	1.00	43.27	N
ATOM	1874	CA	LYS	A	247	65.127	-7.848	26.531	1.00	43.94	C
ATOM	1875	CB	LYS	A	247	65.096	-6.441	25.942	1.00	43.06	C
ATOM	1876	CG	LYS	A	247	66.178	-6.245	24.903	1.00	42.69	C
ATOM	1877	CD	LYS	A	247	66.700	-4.833	24.890	1.00	44.18	C
ATOM	1878	CE	LYS	A	247	67.919	-4.645	25.804	1.00	45.69	C
ATOM	1879	NZ	LYS	A	247	67.868	-3.402	26.674	1.00	45.18	N
ATOM	1880	C	LYS	A	247	64.306	-7.988	27.840	1.00	45.15	C
ATOM	1881	O	LYS	A	247	64.516	-7.266	28.858	1.00	45.19	O
ATOM	1882	N	LEU	A	248	63.396	-8.960	27.807	1.00	46.36	N
ATOM	1883	CA	LEU	A	248	62.555	-9.273	28.950	1.00	47.83	C
ATOM	1884	CB	LEU	A	248	61.090	-9.618	28.541	1.00	47.18	C
ATOM	1885	CG	LEU	A	248	59.873	-8.746	28.944	1.00	43.25	C
ATOM	1886	CD1	LEU	A	248	58.762	-9.605	29.441	1.00	38.49	C
ATOM	1887	CD2	LEU	A	248	60.189	-7.675	29.975	1.00	39.57	C
ATOM	1888	C	LEU	A	248	63.241	-10.424	29.650	1.00	49.64	C
ATOM	1889	O	LEU	A	248	63.508	-10.342	30.861	1.00	50.33	O
ATOM	1890	N	MET	A	249	63.540	-11.486	28.890	1.00	51.29	N
ATOM	1891	CA	MET	A	249	64.421	-12.558	29.384	1.00	52.68	C
ATOM	1892	CB	MET	A	249	64.868	-13.525	28.265	1.00	53.01	C
ATOM	1893	CG	MET	A	249	64.165	-14.929	28.307	1.00	55.23	C
ATOM	1894	SD	MET	A	249	64.329	-15.912	26.739	1.00	58.46	S
ATOM	1895	CE	MET	A	249	65.097	-14.527	25.545	1.00	54.83	C
ATOM	1896	C	MET	A	249	65.622	-11.914	30.077	1.00	52.67	C
ATOM	1897	O	MET	A	249	65.884	-12.220	31.235	1.00	52.62	O
ATOM	1898	N	ASN	A	250	66.290	-10.979	29.392	1.00	53.09	N
ATOM	1899	CA	ASN	A	250	67.403	-10.245	29.964	1.00	53.69	C
ATOM	1900	CB	ASN	A	250	67.891	-9.130	29.045	1.00	53.83	C
ATOM	1901	CG	ASN	A	250	69.152	-8.441	29.575	1.00	55.64	C

235/396

Figure 3A-35

ATOM	1902	OD1	ASN	A	250	70.254	-8.941	29.385	1.00	60.08	O
ATOM	1903	ND2	ASN	A	250	68.993	-7.310	30.262	1.00	55.81	N
ATOM	1904	C	ASN	A	250	67.056	-9.645	31.301	1.00	54.26	C
ATOM	1905	O	ASN	A	250	67.973	-9.243	32.008	1.00	54.69	O
ATOM	1906	N	ALA	A	251	65.754	-9.581	31.654	1.00	54.81	N
ATOM	1907	CA	ALA	A	251	65.303	-9.004	32.958	1.00	54.73	C
ATOM	1908	CB	ALA	A	251	65.047	-7.453	32.823	1.00	54.38	C
ATOM	1909	C	ALA	A	251	64.187	-9.705	33.806	1.00	54.34	C
ATOM	1910	O	ALA	A	251	63.814	-9.212	34.867	1.00	54.36	O
ATOM	1911	N	TYR	A	252	63.692	-10.856	33.369	1.00	54.27	N
ATOM	1912	CA	TYR	A	252	62.816	-11.687	34.208	1.00	55.01	C
ATOM	1913	CB	TYR	A	252	61.344	-11.500	33.823	1.00	55.53	C
ATOM	1914	CG	TYR	A	252	60.747	-10.210	34.343	1.00	56.77	C
ATOM	1915	CD1	TYR	A	252	60.062	-10.159	35.567	1.00	57.20	C
ATOM	1916	CE1	TYR	A	252	59.534	-8.970	36.039	1.00	56.75	C
ATOM	1917	CZ	TYR	A	252	59.700	-7.824	35.285	1.00	57.42	C
ATOM	1918	OH	TYR	A	252	59.206	-6.624	35.683	1.00	59.38	O
ATOM	1919	CE2	TYR	A	252	60.356	-7.851	34.090	1.00	57.54	C
ATOM	1920	CD2	TYR	A	252	60.875	-9.037	33.620	1.00	57.67	C
ATOM	1921	C	TYR	A	252	63.201	-13.168	34.095	1.00	55.31	C
ATOM	1922	O	TYR	A	252	62.335	-14.044	33.860	1.00	54.60	O
ATOM	1923	N	PRO	A	253	64.498	-13.445	34.302	1.00	55.75	N
ATOM	1924	CA	PRO	A	253	65.129	-14.648	33.739	1.00	55.92	C
ATOM	1925	CB	PRO	A	253	66.626	-14.408	33.978	1.00	55.59	C
ATOM	1926	CG	PRO	A	253	66.715	-13.421	35.099	1.00	55.05	C
ATOM	1927	CD	PRO	A	253	65.433	-12.679	35.155	1.00	55.50	C
ATOM	1928	C	PRO	A	253	64.674	-15.921	34.429	1.00	56.42	C
ATOM	1929	O	PRO	A	253	64.229	-15.885	35.564	1.00	56.01	O
ATOM	1930	N	SER	A	254	64.800	-17.043	33.728	1.00	57.66	N
ATOM	1931	CA	SER	A	254	64.448	-18.380	34.246	1.00	58.31	C
ATOM	1932	CB	SER	A	254	64.909	-18.561	35.688	1.00	58.07	C
ATOM	1933	OG	SER	A	254	64.207	-17.678	36.526	1.00	56.05	O
ATOM	1934	C	SER	A	254	62.942	-18.558	34.154	1.00	59.21	C
ATOM	1935	O	SER	A	254	62.397	-19.658	34.403	1.00	59.29	O
ATOM	1936	N	TYR	A	255	62.293	-17.455	33.753	1.00	59.89	N
ATOM	1937	CA	TYR	A	255	60.839	-17.322	33.816	1.00	59.62	C
ATOM	1938	CB	TYR	A	255	60.423	-15.955	34.403	1.00	59.38	C
ATOM	1939	CG	TYR	A	255	60.279	-16.020	35.914	1.00	58.45	C
ATOM	1940	CD1	TYR	A	255	60.908	-15.093	36.742	1.00	57.03	C
ATOM	1941	CE1	TYR	A	255	60.802	-15.182	38.132	1.00	56.46	C
ATOM	1942	CZ	TYR	A	255	60.053	-16.209	38.699	1.00	57.09	C
ATOM	1943	OH	TYR	A	255	59.917	-16.298	40.066	1.00	57.87	O
ATOM	1944	CE2	TYR	A	255	59.429	-17.151	37.902	1.00	57.86	C
ATOM	1945	CD2	TYR	A	255	59.552	-17.060	36.516	1.00	58.43	C
ATOM	1946	C	TYR	A	255	60.136	-17.657	32.508	1.00	59.50	C
ATOM	1947	O	TYR	A	255	59.237	-18.498	32.518	1.00	60.02	O
ATOM	1948	N	ILE	A	256	60.561	-17.052	31.396	1.00	58.99	N
ATOM	1949	CA	ILE	A	256	59.862	-17.247	30.120	1.00	58.29	C
ATOM	1950	CB	ILE	A	256	59.243	-15.914	29.634	1.00	58.58	C
ATOM	1951	CG1	ILE	A	256	58.494	-15.200	30.782	1.00	56.68	C
ATOM	1952	CD1	ILE	A	256	58.962	-13.793	31.048	1.00	53.15	C
ATOM	1953	CG2	ILE	A	256	58.383	-16.143	28.354	1.00	59.16	C
ATOM	1954	C	ILE	A	256	60.680	-17.944	29.000	1.00	58.13	C
ATOM	1955	O	ILE	A	256	61.811	-17.518	28.633	1.00	58.08	O
ATOM	1956	N	SER	A	257	60.080	-19.012	28.473	1.00	57.46	N
ATOM	1957	CA	SER	A	257	60.667	-19.824	27.411	1.00	57.42	C

236/396

Figure 3A-36

ATOM	1958	CB	SER	A	257	59.711	-20.969	27.050	1.00	57.26	C
ATOM	1959	OG	SER	A	257	60.080	-21.652	25.865	1.00	57.63	O
ATOM	1960	C	SER	A	257	60.971	-18.974	26.177	1.00	57.15	C
ATOM	1961	O	SER	A	257	60.103	-18.257	25.694	1.00	57.96	O
ATOM	1962	N	PRO	A	258	62.189	-19.034	25.657	1.00	56.65	N
ATOM	1963	CA	PRO	A	258	62.519	-18.303	24.422	1.00	55.90	C
ATOM	1964	CB	PRO	A	258	64.044	-18.300	24.393	1.00	56.26	C
ATOM	1965	CG	PRO	A	258	64.454	-18.878	25.734	1.00	57.52	C
ATOM	1966	CD	PRO	A	258	63.333	-19.781	26.189	1.00	57.00	C
ATOM	1967	C	PRO	A	258	61.934	-19.030	23.234	1.00	54.74	C
ATOM	1968	O	PRO	A	258	62.513	-19.090	22.145	1.00	53.93	O
ATOM	1969	N	ILE	A	259	60.762	-19.601	23.498	1.00	54.13	N
ATOM	1970	CA	ILE	A	259	59.846	-20.102	22.465	1.00	53.60	C
ATOM	1971	CB	ILE	A	259	60.334	-21.538	21.902	1.00	53.33	C
ATOM	1972	CG1	ILE	A	259	60.079	-21.655	20.398	1.00	51.56	C
ATOM	1973	CD1	ILE	A	259	60.389	-22.995	19.856	1.00	49.88	C
ATOM	1974	CG2	ILE	A	259	59.798	-22.740	22.737	1.00	53.27	C
ATOM	1975	C	ILE	A	259	58.298	-19.937	22.811	1.00	53.10	C
ATOM	1976	O	ILE	A	259	57.465	-19.834	21.902	1.00	52.85	O
ATOM	1977	N	GLY	A	260	57.952	-19.838	24.101	1.00	52.42	N
ATOM	1978	CA	GLY	A	260	56.562	-19.744	24.544	1.00	52.14	C
ATOM	1979	C	GLY	A	260	56.016	-18.355	24.819	1.00	51.98	C
ATOM	1980	O	GLY	A	260	56.758	-17.471	25.228	1.00	51.56	O
ATOM	1981	N	CYS	A	261	54.708	-18.182	24.603	1.00	52.29	N
ATOM	1982	CA	CYS	A	261	53.991	-16.878	24.648	1.00	52.56	C
ATOM	1983	CB	CYS	A	261	52.481	-17.127	24.591	1.00	52.53	C
ATOM	1984	SG	CYS	A	261	51.778	-17.716	23.040	1.00	54.52	S
ATOM	1985	C	CYS	A	261	54.216	-16.034	25.906	1.00	52.41	C
ATOM	1986	O	CYS	A	261	53.971	-16.513	27.024	1.00	53.06	O
ATOM	1987	N	LEU	A	262	54.624	-14.774	25.764	1.00	51.61	N
ATOM	1988	CA	LEU	A	262	54.864	-13.954	26.962	1.00	50.56	C
ATOM	1989	CB	LEU	A	262	54.934	-12.493	26.584	1.00	49.77	C
ATOM	1990	CG	LEU	A	262	56.301	-12.074	26.115	1.00	48.04	C
ATOM	1991	CD1	LEU	A	262	56.200	-11.088	24.994	1.00	46.94	C
ATOM	1992	CD2	LEU	A	262	57.000	-11.461	27.275	1.00	48.28	C
ATOM	1993	C	LEU	A	262	53.811	-14.179	28.073	1.00	50.82	C
ATOM	1994	O	LEU	A	262	52.629	-14.239	27.810	1.00	50.54	O
ATOM	1995	N	PRO	A	263	54.226	-14.357	29.313	1.00	51.56	N
ATOM	1996	CA	PRO	A	263	53.254	-14.442	30.406	1.00	52.28	C
ATOM	1997	CB	PRO	A	263	54.130	-14.815	31.615	1.00	52.61	C
ATOM	1998	CG	PRO	A	263	55.503	-14.244	31.291	1.00	52.09	C
ATOM	1999	CD	PRO	A	263	55.609	-14.495	29.805	1.00	52.04	C
ATOM	2000	C	PRO	A	263	52.530	-13.083	30.601	1.00	52.48	C
ATOM	2001	O	PRO	A	263	53.164	-12.019	30.510	1.00	52.80	O
ATOM	2002	N	ALA	A	264	51.234	-13.124	30.897	1.00	52.17	N
ATOM	2003	CA	ALA	A	264	50.364	-11.962	30.676	1.00	52.06	C
ATOM	2004	CB	ALA	A	264	48.912	-12.380	30.687	1.00	52.54	C
ATOM	2005	C	ALA	A	264	50.525	-10.764	31.584	1.00	51.94	C
ATOM	2006	O	ALA	A	264	49.760	-9.798	31.468	1.00	51.81	O
ATOM	2007	N	HIS	A	265	51.481	-10.801	32.492	1.00	51.53	N
ATOM	2008	CA	HIS	A	265	51.517	-9.737	33.459	1.00	51.59	C
ATOM	2009	CB	HIS	A	265	51.413	-10.328	34.834	1.00	51.52	C
ATOM	2010	CG	HIS	A	265	52.362	-11.439	35.055	1.00	51.81	C
ATOM	2011	ND1	HIS	A	265	52.808	-12.234	34.026	1.00	51.70	N
ATOM	2012	CE1	HIS	A	265	53.656	-13.123	34.509	1.00	54.22	C
ATOM	2013	NE2	HIS	A	265	53.770	-12.933	35.813	1.00	54.66	N

237/396

Figure 3A-37

ATOM	2014	CD2	HIS	A	265	52.984	-11.872	36.176	1.00	53.30	C
ATOM	2015	C	HIS	A	265	52.767	-8.904	33.364	1.00	51.78	C
ATOM	2016	O	HIS	A	265	52.961	-7.977	34.166	1.00	52.24	O
ATOM	2017	N	LEU	A	266	53.628	-9.215	32.398	1.00	51.47	N
ATOM	2018	CA	LEU	A	266	54.920	-8.530	32.360	1.00	50.85	C
ATOM	2019	CB	LEU	A	266	56.117	-9.516	32.275	1.00	51.10	C
ATOM	2020	CG	LEU	A	266	56.336	-10.566	33.413	1.00	52.41	C
ATOM	2021	CD1	LEU	A	266	57.674	-11.358	33.302	1.00	50.91	C
ATOM	2022	CD2	LEU	A	266	56.112	-10.034	34.904	1.00	52.24	C
ATOM	2023	C	LEU	A	266	54.964	-7.486	31.272	1.00	49.94	C
ATOM	2024	O	LEU	A	266	55.979	-6.802	31.135	1.00	50.30	O
ATOM	2025	N	LEU	A	267	53.856	-7.329	30.542	1.00	48.29	N
ATOM	2026	CA	LEU	A	267	53.886	-6.592	29.291	1.00	46.59	C
ATOM	2027	CB	LEU	A	267	52.954	-7.190	28.275	1.00	46.01	C
ATOM	2028	CG	LEU	A	267	53.051	-8.649	27.959	1.00	45.52	C
ATOM	2029	CD1	LEU	A	267	51.635	-9.129	27.754	1.00	45.73	C
ATOM	2030	CD2	LEU	A	267	53.857	-8.824	26.717	1.00	44.69	C
ATOM	2031	C	LEU	A	267	53.521	-5.151	29.382	1.00	46.13	C
ATOM	2032	O	LEU	A	267	53.354	-4.540	28.330	1.00	46.30	O
ATOM	2033	N	GLY	A	268	53.350	-4.605	30.586	1.00	45.33	N
ATOM	2034	CA	GLY	A	268	53.226	-3.152	30.725	1.00	45.22	C
ATOM	2035	C	GLY	A	268	51.995	-2.472	31.362	1.00	44.85	C
ATOM	2036	O	GLY	A	268	52.081	-1.291	31.833	1.00	44.71	O
ATOM	2037	N	ASP	A	269	50.859	-3.185	31.354	1.00	43.90	N
ATOM	2038	CA	ASP	A	269	49.667	-2.806	32.142	1.00	43.05	C
ATOM	2039	CB	ASP	A	269	48.798	-1.786	31.404	1.00	43.08	C
ATOM	2040	CG	ASP	A	269	48.675	-2.109	29.924	1.00	43.47	C
ATOM	2041	OD1	ASP	A	269	48.746	-1.156	29.093	1.00	44.31	O
ATOM	2042	OD2	ASP	A	269	48.532	-3.293	29.515	1.00	41.63	O
ATOM	2043	C	ASP	A	269	48.859	-4.056	32.502	1.00	41.97	C
ATOM	2044	O	ASP	A	269	49.305	-5.187	32.268	1.00	41.45	O
ATOM	2045	N	MET	A	270	47.672	-3.838	33.060	1.00	40.70	N
ATOM	2046	CA	MET	A	270	46.885	-4.912	33.645	1.00	39.61	C
ATOM	2047	CB	MET	A	270	45.811	-4.311	34.536	1.00	39.56	C
ATOM	2048	CG	MET	A	270	44.673	-5.221	34.812	1.00	41.54	C
ATOM	2049	SD	MET	A	270	44.997	-6.446	36.113	1.00	45.26	S
ATOM	2050	CE	MET	A	270	44.961	-5.196	37.579	1.00	44.79	C
ATOM	2051	C	MET	A	270	46.318	-5.902	32.610	1.00	38.78	C
ATOM	2052	O	MET	A	270	45.921	-7.029	32.954	1.00	38.50	O
ATOM	2053	N	TRP	A	271	46.327	-5.499	31.339	1.00	38.01	N
ATOM	2054	CA	TRP	A	271	45.906	-6.387	30.244	1.00	37.13	C
ATOM	2055	CB	TRP	A	271	44.556	-5.945	29.614	1.00	37.31	C
ATOM	2056	CG	TRP	A	271	43.694	-5.378	30.647	1.00	36.16	C
ATOM	2057	CD1	TRP	A	271	42.735	-6.020	31.370	1.00	34.98	C
ATOM	2058	NE1	TRP	A	271	42.204	-5.164	32.304	1.00	35.74	N
ATOM	2059	CE2	TRP	A	271	42.841	-3.955	32.203	1.00	36.85	C
ATOM	2060	CD2	TRP	A	271	43.783	-4.062	31.157	1.00	36.13	C
ATOM	2061	CE3	TRP	A	271	44.571	-2.944	30.831	1.00	35.68	C
ATOM	2062	CZ3	TRP	A	271	44.392	-1.778	31.536	1.00	37.31	C
ATOM	2063	CH2	TRP	A	271	43.442	-1.695	32.586	1.00	38.16	C
ATOM	2064	CZ2	TRP	A	271	42.663	-2.777	32.935	1.00	38.17	C
ATOM	2065	C	TRP	A	271	46.976	-6.627	29.175	1.00	36.44	C
ATOM	2066	O	TRP	A	271	46.902	-7.640	28.470	1.00	37.12	O
ATOM	2067	N	GLY	A	272	47.957	-5.727	29.056	1.00	35.06	N
ATOM	2068	CA	GLY	A	272	49.002	-5.875	28.050	1.00	34.08	C
ATOM	2069	C	GLY	A	272	48.615	-5.257	26.721	1.00	33.45	C

238/396

Figure 3A-38

ATOM	2070	O	GLY	A	272	49.035	-5.657	25.628	1.00	33.16	O
ATOM	2071	N	ARG	A	273	47.772	-4.258	26.835	1.00	33.21	N
ATOM	2072	CA	ARG	A	273	47.122	-3.683	25.694	1.00	33.06	C
ATOM	2073	CB	ARG	A	273	45.854	-2.993	26.178	1.00	32.44	C
ATOM	2074	CG	ARG	A	273	45.770	-1.522	25.991	1.00	30.42	C
ATOM	2075	CD	ARG	A	273	44.326	-1.049	26.007	1.00	30.56	C
ATOM	2076	NE	ARG	A	273	43.812	-0.781	24.664	1.00	26.76	N
ATOM	2077	CZ	ARG	A	273	42.985	0.203	24.349	1.00	22.31	C
ATOM	2078	NH1	ARG	A	273	42.650	0.301	23.088	1.00	21.63	N
ATOM	2079	NH2	ARG	A	273	42.503	1.064	25.258	1.00	16.35	N
ATOM	2080	C	ARG	A	273	48.119	-2.745	25.051	1.00	33.88	C
ATOM	2081	O	ARG	A	273	48.254	-2.709	23.828	1.00	33.97	O
ATOM	2082	N	PHE	A	274	48.821	-2.002	25.902	1.00	34.47	N
ATOM	2083	CA	PHE	A	274	49.998	-1.284	25.506	1.00	35.04	C
ATOM	2084	CB	PHE	A	274	49.900	0.170	25.906	1.00	35.25	C
ATOM	2085	CG	PHE	A	274	48.548	0.780	25.657	1.00	39.86	C
ATOM	2086	CD1	PHE	A	274	47.779	1.280	26.715	1.00	42.88	C
ATOM	2087	CE1	PHE	A	274	46.486	1.875	26.466	1.00	43.18	C
ATOM	2088	CZ	PHE	A	274	45.975	1.963	25.161	1.00	41.36	C
ATOM	2089	CE2	PHE	A	274	46.727	1.461	24.108	1.00	42.08	C
ATOM	2090	CD2	PHE	A	274	48.021	0.872	24.355	1.00	43.12	C
ATOM	2091	C	PHE	A	274	51.161	-1.960	26.210	1.00	34.91	C
ATOM	2092	O	PHE	A	274	51.264	-1.926	27.425	1.00	35.44	O
ATOM	2093	N	TRP	A	275	51.996	-2.631	25.423	1.00	34.50	N
ATOM	2094	CA	TRP	A	275	53.371	-2.919	25.756	1.00	33.64	C
ATOM	2095	CB	TRP	A	275	53.940	-3.684	24.612	1.00	32.36	C
ATOM	2096	CG	TRP	A	275	53.414	-4.931	24.555	1.00	28.95	C
ATOM	2097	CD1	TRP	A	275	52.497	-5.465	25.396	1.00	28.28	C
ATOM	2098	NE1	TRP	A	275	52.213	-6.762	25.025	1.00	28.25	N
ATOM	2099	CE2	TRP	A	275	52.976	-7.080	23.938	1.00	25.89	C
ATOM	2100	CD2	TRP	A	275	53.758	-5.933	23.626	1.00	25.84	C
ATOM	2101	CE3	TRP	A	275	54.638	-5.988	22.550	1.00	21.91	C
ATOM	2102	CZ3	TRP	A	275	54.692	-7.137	21.825	1.00	23.08	C
ATOM	2103	CH2	TRP	A	275	53.904	-8.268	22.159	1.00	23.18	C
ATOM	2104	CZ2	TRP	A	275	53.040	-8.250	23.211	1.00	24.32	C
ATOM	2105	C	TRP	A	275	54.252	-1.686	25.818	1.00	35.03	C
ATOM	2106	O	TRP	A	275	55.363	-1.715	25.295	1.00	35.27	O
ATOM	2107	N	THR	A	276	53.804	-0.598	26.420	1.00	36.11	N
ATOM	2108	CA	THR	A	276	54.579	0.616	26.270	1.00	37.32	C
ATOM	2109	CB	THR	A	276	53.663	1.862	26.144	1.00	37.78	C
ATOM	2110	OG1	THR	A	276	54.464	3.052	26.209	1.00	40.22	O
ATOM	2111	CG2	THR	A	276	52.638	1.988	27.338	1.00	38.47	C
ATOM	2112	C	THR	A	276	55.687	0.695	27.342	1.00	37.37	C
ATOM	2113	O	THR	A	276	56.794	0.223	27.079	1.00	37.71	O
ATOM	2114	N	ASN	A	277	55.383	1.271	28.510	1.00	37.23	N
ATOM	2115	CA	ASN	A	277	56.143	1.140	29.758	1.00	37.43	C
ATOM	2116	CB	ASN	A	277	55.168	0.989	30.946	1.00	38.40	C
ATOM	2117	CG	ASN	A	277	54.449	2.317	31.325	1.00	41.23	C
ATOM	2118	OD1	ASN	A	277	53.213	2.346	31.433	1.00	44.78	O
ATOM	2119	ND2	ASN	A	277	55.218	3.403	31.543	1.00	43.19	N
ATOM	2120	C	ASN	A	277	57.232	0.033	29.838	1.00	36.84	C
ATOM	2121	O	ASN	A	277	58.333	0.261	30.364	1.00	37.59	O
ATOM	2122	N	LEU	A	278	56.949	-1.163	29.346	1.00	35.18	N
ATOM	2123	CA	LEU	A	278	58.021	-2.077	29.032	1.00	33.40	C
ATOM	2124	CB	LEU	A	278	57.495	-3.125	28.050	1.00	32.77	C
ATOM	2125	CG	LEU	A	278	57.335	-4.626	28.352	1.00	31.45	C

239/396

Figure 3A-39

ATOM	2126	CD1	LEU	A	278	56.445	-4.870	29.537	1.00	30.63	C
ATOM	2127	CD2	LEU	A	278	56.808	-5.421	27.184	1.00	26.92	C
ATOM	2128	C	LEU	A	278	59.109	-1.360	28.283	1.00	33.45	C
ATOM	2129	O	LEU	A	278	59.721	-1.987	27.499	1.00	34.02	O
ATOM	2130	N	TYR	A	279	59.342	-0.061	28.450	1.00	34.03	N
ATOM	2131	CA	TYR	A	279	60.361	0.659	27.649	1.00	34.76	C
ATOM	2132	CB	TYR	A	279	60.091	2.168	27.554	1.00	33.81	C
ATOM	2133	CG	TYR	A	279	61.022	2.898	26.582	1.00	30.81	C
ATOM	2134	CD1	TYR	A	279	61.338	2.351	25.324	1.00	27.58	C
ATOM	2135	CE1	TYR	A	279	62.195	2.997	24.461	1.00	26.04	C
ATOM	2136	CZ	TYR	A	279	62.757	4.238	24.828	1.00	27.62	C
ATOM	2137	OH	TYR	A	279	63.631	4.932	23.964	1.00	29.33	O
ATOM	2138	CE2	TYR	A	279	62.460	4.790	26.069	1.00	26.53	C
ATOM	2139	CD2	TYR	A	279	61.595	4.118	26.930	1.00	27.96	C
ATOM	2140	C	TYR	A	279	61.790	0.457	28.162	1.00	37.04	C
ATOM	2141	O	TYR	A	279	62.639	-0.102	27.428	1.00	37.11	O
ATOM	2142	N	SER	A	280	62.050	0.980	29.381	1.00	39.12	N
ATOM	2143	CA	SER	A	280	63.168	0.594	30.278	1.00	40.72	C
ATOM	2144	CB	SER	A	280	62.730	0.611	31.759	1.00	41.10	C
ATOM	2145	OG	SER	A	280	62.526	1.926	32.288	1.00	42.82	O
ATOM	2146	C	SER	A	280	63.652	-0.820	29.979	1.00	41.38	C
ATOM	2147	O	SER	A	280	64.817	-1.004	29.626	1.00	42.14	O
ATOM	2148	N	LEU	A	281	62.770	-1.815	30.098	1.00	41.42	N
ATOM	2149	CA	LEU	A	281	63.134	-3.162	29.667	1.00	42.23	C
ATOM	2150	CB	LEU	A	281	62.111	-4.208	30.132	1.00	41.79	C
ATOM	2151	CG	LEU	A	281	62.067	-4.485	31.626	1.00	41.31	C
ATOM	2152	CD1	LEU	A	281	62.191	-3.175	32.419	1.00	42.02	C
ATOM	2153	CD2	LEU	A	281	60.809	-5.219	32.006	1.00	39.22	C
ATOM	2154	C	LEU	A	281	63.486	-3.384	28.161	1.00	43.32	C
ATOM	2155	O	LEU	A	281	63.976	-4.483	27.844	1.00	44.48	O
ATOM	2156	N	THR	A	282	63.286	-2.404	27.253	1.00	43.44	N
ATOM	2157	CA	THR	A	282	63.540	-2.630	25.809	1.00	43.91	C
ATOM	2158	CB	THR	A	282	62.234	-2.840	25.066	1.00	43.78	C
ATOM	2159	OG1	THR	A	282	61.357	-1.780	25.427	1.00	44.50	O
ATOM	2160	CG2	THR	A	282	61.501	-4.082	25.538	1.00	43.77	C
ATOM	2161	C	THR	A	282	64.322	-1.560	25.041	1.00	44.70	C
ATOM	2162	O	THR	A	282	64.720	-1.797	23.882	1.00	44.19	O
ATOM	2163	N	VAL	A	283	64.497	-0.381	25.650	1.00	46.16	N
ATOM	2164	CA	VAL	A	283	65.296	0.712	25.056	1.00	47.64	C
ATOM	2165	CB	VAL	A	283	65.691	1.830	26.113	1.00	46.90	C
ATOM	2166	CG1	VAL	A	283	66.534	1.288	27.206	1.00	47.07	C
ATOM	2167	CG2	VAL	A	283	66.377	3.015	25.488	1.00	45.30	C
ATOM	2168	C	VAL	A	283	66.507	0.068	24.398	1.00	49.76	C
ATOM	2169	O	VAL	A	283	67.224	-0.678	25.049	1.00	50.19	O
ATOM	2170	N	PRO	A	284	66.726	0.296	23.107	1.00	52.03	N
ATOM	2171	CA	PRO	A	284	67.758	-0.471	22.380	1.00	53.83	C
ATOM	2172	CB	PRO	A	284	67.289	-0.362	20.912	1.00	53.78	C
ATOM	2173	CG	PRO	A	284	66.673	1.065	20.834	1.00	53.31	C
ATOM	2174	CD	PRO	A	284	66.078	1.304	22.238	1.00	52.41	C
ATOM	2175	C	PRO	A	284	69.232	0.060	22.584	1.00	55.18	C
ATOM	2176	O	PRO	A	284	70.217	-0.722	22.531	1.00	55.45	O
ATOM	2177	N	PHE	A	285	69.352	1.375	22.791	1.00	56.03	N
ATOM	2178	CA	PHE	A	285	70.607	2.038	23.036	1.00	57.17	C
ATOM	2179	CB	PHE	A	285	71.028	2.905	21.859	1.00	57.44	C
ATOM	2180	CG	PHE	A	285	71.087	2.184	20.541	1.00	59.65	C
ATOM	2181	CD1	PHE	A	285	70.075	2.363	19.585	1.00	62.17	C

240/396

Figure 3A-40

ATOM	2182	CE1	PHE	A	285	70.123	1.709	18.330	1.00	63.13	C
ATOM	2183	CZ	PHE	A	285	71.206	0.888	18.022	1.00	63.88	C
ATOM	2184	CE2	PHE	A	285	72.230	0.707	18.973	1.00	64.02	C
ATOM	2185	CD2	PHE	A	285	72.163	1.357	20.227	1.00	61.82	C
ATOM	2186	C	PHE	A	285	70.269	2.922	24.190	1.00	57.86	C
ATOM	2187	O	PHE	A	285	70.265	4.158	24.066	1.00	57.49	O
ATOM	2188	N	GLY	A	286	69.996	2.264	25.318	1.00	59.30	N
ATOM	2189	CA	GLY	A	286	69.491	2.880	26.539	1.00	61.12	C
ATOM	2190	C	GLY	A	286	70.131	4.111	27.180	1.00	62.23	C
ATOM	2191	O	GLY	A	286	69.850	4.380	28.361	1.00	62.46	O
ATOM	2192	N	GLN	A	287	70.931	4.882	26.430	1.00	63.05	N
ATOM	2193	CA	GLN	A	287	71.779	5.900	27.063	1.00	63.75	C
ATOM	2194	CB	GLN	A	287	73.154	5.326	27.457	1.00	63.77	C
ATOM	2195	CG	GLN	A	287	73.596	4.106	26.660	1.00	64.11	C
ATOM	2196	CD	GLN	A	287	73.948	4.404	25.191	1.00	64.07	C
ATOM	2197	OE1	GLN	A	287	74.026	5.570	24.759	1.00	63.76	O
ATOM	2198	NE2	GLN	A	287	74.171	3.331	24.423	1.00	63.12	N
ATOM	2199	C	GLN	A	287	72.000	7.229	26.368	1.00	64.14	C
ATOM	2200	O	GLN	A	287	72.962	7.907	26.732	1.00	64.50	O
ATOM	2201	N	LYS	A	288	71.163	7.616	25.395	1.00	64.49	N
ATOM	2202	CA	LYS	A	288	71.043	9.053	25.040	1.00	64.73	C
ATOM	2203	CB	LYS	A	288	70.872	9.277	23.532	1.00	64.17	C
ATOM	2204	CG	LYS	A	288	71.717	8.373	22.651	1.00	63.46	C
ATOM	2205	CD	LYS	A	288	72.973	9.061	22.140	1.00	62.62	C
ATOM	2206	CE	LYS	A	288	73.971	8.019	21.574	1.00	63.07	C
ATOM	2207	NZ	LYS	A	288	73.698	7.605	20.144	1.00	59.99	N
ATOM	2208	C	LYS	A	288	69.873	9.619	25.873	1.00	65.61	C
ATOM	2209	O	LYS	A	288	69.262	8.849	26.635	1.00	66.04	O
ATOM	2210	N	PRO	A	289	69.550	10.918	25.793	1.00	66.25	N
ATOM	2211	CA	PRO	A	289	68.425	11.459	26.591	1.00	66.51	C
ATOM	2212	CB	PRO	A	289	68.339	12.937	26.174	1.00	66.53	C
ATOM	2213	CG	PRO	A	289	69.699	13.259	25.638	1.00	67.14	C
ATOM	2214	CD	PRO	A	289	70.205	11.969	24.996	1.00	66.69	C
ATOM	2215	C	PRO	A	289	67.088	10.751	26.322	1.00	66.42	C
ATOM	2216	O	PRO	A	289	66.737	10.523	25.153	1.00	66.48	O
ATOM	2217	N	ASN	A	290	66.390	10.392	27.407	1.00	66.04	N
ATOM	2218	CA	ASN	A	290	65.087	9.755	27.353	1.00	65.29	C
ATOM	2219	CB	ASN	A	290	64.489	9.544	28.765	1.00	65.09	C
ATOM	2220	CG	ASN	A	290	64.179	8.055	29.084	1.00	65.37	C
ATOM	2221	OD1	ASN	A	290	64.077	7.661	30.247	1.00	64.31	O
ATOM	2222	ND2	ASN	A	290	64.037	7.235	28.047	1.00	67.32	N
ATOM	2223	C	ASN	A	290	64.167	10.620	26.518	1.00	65.28	C
ATOM	2224	O	ASN	A	290	64.130	11.861	26.674	1.00	65.39	O
ATOM	2225	N	ILE	A	291	63.508	9.942	25.574	1.00	64.74	N
ATOM	2226	CA	ILE	A	291	62.293	10.394	24.904	1.00	63.57	C
ATOM	2227	CB	ILE	A	291	62.430	10.136	23.405	1.00	63.67	C
ATOM	2228	CG1	ILE	A	291	63.121	11.342	22.756	1.00	63.65	C
ATOM	2229	CD1	ILE	A	291	64.591	11.118	22.449	1.00	63.90	C
ATOM	2230	CG2	ILE	A	291	61.065	9.762	22.751	1.00	63.46	C
ATOM	2231	C	ILE	A	291	61.173	9.569	25.530	1.00	62.86	C
ATOM	2232	O	ILE	A	291	60.334	8.957	24.849	1.00	62.92	O
ATOM	2233	N	ASP	A	292	61.263	9.496	26.850	1.00	61.64	N
ATOM	2234	CA	ASP	A	292	60.246	8.998	27.726	1.00	61.08	C
ATOM	2235	CB	ASP	A	292	60.646	7.662	28.356	1.00	61.08	C
ATOM	2236	CG	ASP	A	292	59.581	7.098	29.325	1.00	61.93	C
ATOM	2237	OD1	ASP	A	292	59.491	5.864	29.471	1.00	62.63	O

241/396

Figure 3A-41

ATOM	2238	OD2	ASP	A	292	58.798	7.787	30.011	1.00	63.36	O
ATOM	2239	C	ASP	A	292	60.322	10.133	28.714	1.00	60.83	C
ATOM	2240	O	ASP	A	292	60.696	9.957	29.884	1.00	60.66	O
ATOM	2241	N	VAL	A	293	59.991	11.319	28.207	1.00	60.49	N
ATOM	2242	CA	VAL	A	293	60.038	12.553	28.980	1.00	60.60	C
ATOM	2243	CB	VAL	A	293	59.601	13.735	28.141	1.00	60.55	C
ATOM	2244	CG1	VAL	A	293	60.667	14.823	28.211	1.00	61.24	C
ATOM	2245	CG2	VAL	A	293	59.361	13.304	26.705	1.00	60.46	C
ATOM	2246	C	VAL	A	293	59.218	12.550	30.263	1.00	60.76	C
ATOM	2247	O	VAL	A	293	58.774	13.610	30.724	1.00	60.38	O
ATOM	2248	N	THR	A	294	59.050	11.357	30.849	1.00	61.24	N
ATOM	2249	CA	THR	A	294	58.219	11.188	32.043	1.00	61.65	C
ATOM	2250	CB	THR	A	294	57.813	9.710	32.327	1.00	61.38	C
ATOM	2251	OG1	THR	A	294	57.154	9.654	33.601	1.00	60.22	O
ATOM	2252	CG2	THR	A	294	59.029	8.792	32.514	1.00	61.33	C
ATOM	2253	C	THR	A	294	58.852	11.786	33.269	1.00	62.37	C
ATOM	2254	O	THR	A	294	58.135	12.348	34.088	1.00	62.66	O
ATOM	2255	N	ASP	A	295	60.184	11.644	33.367	1.00	63.13	N
ATOM	2256	CA	ASP	A	295	61.021	12.101	34.487	1.00	63.41	C
ATOM	2257	CB	ASP	A	295	62.386	11.360	34.468	1.00	63.91	C
ATOM	2258	CG	ASP	A	295	62.273	9.832	34.732	1.00	65.05	C
ATOM	2259	OD1	ASP	A	295	62.308	9.438	35.929	1.00	66.61	O
ATOM	2260	OD2	ASP	A	295	62.186	8.954	33.821	1.00	64.88	O
ATOM	2261	C	ASP	A	295	61.255	13.609	34.325	1.00	63.24	C
ATOM	2262	O	ASP	A	295	61.097	14.411	35.267	1.00	62.54	O
ATOM	2263	N	ALA	A	296	61.632	13.958	33.096	1.00	63.50	N
ATOM	2264	CA	ALA	A	296	61.896	15.324	32.684	1.00	63.92	C
ATOM	2265	CB	ALA	A	296	62.143	15.374	31.183	1.00	63.84	C
ATOM	2266	C	ALA	A	296	60.738	16.220	33.062	1.00	64.18	C
ATOM	2267	O	ALA	A	296	60.940	17.378	33.428	1.00	64.14	O
ATOM	2268	N	MET	A	297	59.535	15.648	32.979	1.00	64.77	N
ATOM	2269	CA	MET	A	297	58.252	16.316	33.267	1.00	65.17	C
ATOM	2270	CB	MET	A	297	57.090	15.398	32.825	1.00	65.23	C
ATOM	2271	CG	MET	A	297	56.460	15.733	31.466	1.00	64.62	C
ATOM	2272	SD	MET	A	297	55.305	14.459	30.903	1.00	61.60	S
ATOM	2273	CE	MET	A	297	54.140	14.568	32.194	1.00	60.69	C
ATOM	2274	C	MET	A	297	58.083	16.692	34.757	1.00	65.16	C
ATOM	2275	O	MET	A	297	57.830	17.855	35.099	1.00	64.73	O
ATOM	2276	N	VAL	A	298	58.207	15.678	35.616	1.00	65.34	N
ATOM	2277	CA	VAL	A	298	58.138	15.820	37.064	1.00	65.45	C
ATOM	2278	CB	VAL	A	298	58.408	14.483	37.779	1.00	65.17	C
ATOM	2279	CG1	VAL	A	298	58.233	14.658	39.297	1.00	65.45	C
ATOM	2280	CG2	VAL	A	298	57.506	13.380	37.242	1.00	64.60	C
ATOM	2281	C	VAL	A	298	59.198	16.806	37.536	1.00	65.78	C
ATOM	2282	O	VAL	A	298	58.894	17.816	38.207	1.00	66.08	O
ATOM	2283	N	ASP	A	299	60.443	16.504	37.164	1.00	65.54	N
ATOM	2284	CA	ASP	A	299	61.589	17.327	37.545	1.00	65.05	C
ATOM	2285	CB	ASP	A	299	62.915	16.588	37.242	1.00	65.25	C
ATOM	2286	CG	ASP	A	299	63.578	16.046	38.507	1.00	65.64	C
ATOM	2287	OD1	ASP	A	299	64.278	16.844	39.174	1.00	66.16	O
ATOM	2288	OD2	ASP	A	299	63.438	14.864	38.924	1.00	64.74	O
ATOM	2289	C	ASP	A	299	61.556	18.766	36.964	1.00	64.28	C
ATOM	2290	O	ASP	A	299	62.401	19.596	37.342	1.00	64.56	O
ATOM	2291	N	GLN	A	300	60.576	19.059	36.083	1.00	62.86	N
ATOM	2292	CA	GLN	A	300	60.359	20.423	35.545	1.00	60.99	C
ATOM	2293	CB	GLN	A	300	60.386	20.431	34.018	1.00	60.22	C

242/396

Figure 3A-42

ATOM	2294	CG	GLN	A	300	60.404	21.814	33.450	1.00	57.71	C
ATOM	2295	CD	GLN	A	300	60.487	21.838	31.953	1.00	56.69	C
ATOM	2296	OE1	GLN	A	300	61.246	21.064	31.342	1.00	55.65	O
ATOM	2297	NE2	GLN	A	300	59.719	22.739	31.340	1.00	55.73	N
ATOM	2298	C	GLN	A	300	59.127	21.203	36.076	1.00	60.60	C
ATOM	2299	O	GLN	A	300	58.687	22.160	35.437	1.00	59.97	O
ATOM	2300	N	ALA	A	301	58.607	20.807	37.243	1.00	60.27	N
ATOM	2301	CA	ALA	A	301	57.490	21.496	37.909	1.00	60.39	C
ATOM	2302	CB	ALA	A	301	57.417	22.988	37.495	1.00	60.24	C
ATOM	2303	C	ALA	A	301	56.129	20.841	37.703	1.00	60.44	C
ATOM	2304	O	ALA	A	301	55.248	20.930	38.562	1.00	60.41	O
ATOM	2305	N	TRP	A	302	56.019	20.125	36.589	1.00	60.61	N
ATOM	2306	CA	TRP	A	302	54.785	19.918	35.804	1.00	60.46	C
ATOM	2307	CB	TRP	A	302	55.147	19.097	34.557	1.00	60.72	C
ATOM	2308	CG	TRP	A	302	55.396	19.957	33.367	1.00	61.88	C
ATOM	2309	CD1	TRP	A	302	55.926	21.224	33.352	1.00	62.04	C
ATOM	2310	NE1	TRP	A	302	55.980	21.702	32.067	1.00	61.60	N
ATOM	2311	CE2	TRP	A	302	55.455	20.758	31.227	1.00	63.36	C
ATOM	2312	CD2	TRP	A	302	55.076	19.644	32.022	1.00	63.51	C
ATOM	2313	CE3	TRP	A	302	54.498	18.531	31.395	1.00	64.04	C
ATOM	2314	CZ3	TRP	A	302	54.337	18.554	30.018	1.00	65.21	C
ATOM	2315	CH2	TRP	A	302	54.734	19.678	29.250	1.00	64.96	C
ATOM	2316	CZ2	TRP	A	302	55.287	20.786	29.839	1.00	64.44	C
ATOM	2317	C	TRP	A	302	53.483	19.360	36.414	1.00	59.88	C
ATOM	2318	O	TRP	A	302	53.455	18.234	36.903	1.00	60.03	O
ATOM	2319	N	ASP	A	303	52.401	20.134	36.307	1.00	59.02	N
ATOM	2320	CA	ASP	A	303	51.058	19.668	36.661	1.00	58.62	C
ATOM	2321	CB	ASP	A	303	50.410	20.688	37.576	1.00	57.84	C
ATOM	2322	CG	ASP	A	303	50.389	22.022	36.967	1.00	56.48	C
ATOM	2323	OD1	ASP	A	303	49.998	22.981	37.650	1.00	57.33	O
ATOM	2324	OD2	ASP	A	303	50.769	22.208	35.798	1.00	53.07	O
ATOM	2325	C	ASP	A	303	50.095	19.347	35.468	1.00	59.05	C
ATOM	2326	O	ASP	A	303	50.384	19.637	34.294	1.00	59.18	O
ATOM	2327	N	ALA	A	304	48.941	18.751	35.792	1.00	59.06	N
ATOM	2328	CA	ALA	A	304	47.894	18.444	34.811	1.00	58.47	C
ATOM	2329	CB	ALA	A	304	46.651	17.905	35.511	1.00	58.81	C
ATOM	2330	C	ALA	A	304	47.544	19.653	33.952	1.00	58.13	C
ATOM	2331	O	ALA	A	304	47.989	19.718	32.808	1.00	57.65	O
ATOM	2332	N	GLN	A	305	46.769	20.597	34.510	1.00	57.72	N
ATOM	2333	CA	GLN	A	305	46.460	21.881	33.860	1.00	57.88	C
ATOM	2334	CB	GLN	A	305	46.352	22.981	34.909	1.00	58.31	C
ATOM	2335	CG	GLN	A	305	46.387	24.437	34.393	1.00	61.59	C
ATOM	2336	CD	GLN	A	305	45.281	25.335	35.040	1.00	67.16	C
ATOM	2337	OE1	GLN	A	305	44.087	24.945	35.058	1.00	68.86	O
ATOM	2338	NE2	GLN	A	305	45.674	26.529	35.554	1.00	67.00	N
ATOM	2339	C	GLN	A	305	47.520	22.250	32.825	1.00	57.21	C
ATOM	2340	O	GLN	A	305	47.241	22.300	31.639	1.00	57.44	O
ATOM	2341	N	ARG	A	306	48.745	22.475	33.291	1.00	56.50	N
ATOM	2342	CA	ARG	A	306	49.916	22.606	32.438	1.00	55.41	C
ATOM	2343	CB	ARG	A	306	51.176	22.360	33.242	1.00	55.36	C
ATOM	2344	CG	ARG	A	306	52.394	22.290	32.405	1.00	56.82	C
ATOM	2345	CD	ARG	A	306	52.954	23.645	32.102	1.00	60.41	C
ATOM	2346	NE	ARG	A	306	54.054	23.549	31.152	1.00	62.13	N
ATOM	2347	CZ	ARG	A	306	55.217	24.147	31.308	1.00	62.73	C
ATOM	2348	NH1	ARG	A	306	55.435	24.893	32.384	1.00	62.65	N
ATOM	2349	NH2	ARG	A	306	56.166	23.993	30.393	1.00	63.75	N

243/396

Figure 3A-43

ATOM	2350	C	ARG	A	306	49.876	21.664	31.252	1.00	54.49	C
ATOM	2351	O	ARG	A	306	49.889	22.111	30.114	1.00	54.34	O
ATOM	2352	N	ILE	A	307	49.814	20.365	31.500	1.00	53.72	N
ATOM	2353	CA	ILE	A	307	49.677	19.448	30.373	1.00	53.27	C
ATOM	2354	CB	ILE	A	307	49.465	17.966	30.829	1.00	53.37	C
ATOM	2355	CG1	ILE	A	307	50.399	17.592	31.985	1.00	53.39	C
ATOM	2356	CD1	ILE	A	307	50.749	16.084	32.061	1.00	52.83	C
ATOM	2357	CG2	ILE	A	307	49.688	17.012	29.676	1.00	52.36	C
ATOM	2358	C	ILE	A	307	48.538	19.946	29.465	1.00	52.75	C
ATOM	2359	O	ILE	A	307	48.750	20.244	28.306	1.00	52.22	O
ATOM	2360	N	PHE	A	308	47.349	20.087	30.021	1.00	52.55	N
ATOM	2361	CA	PHE	A	308	46.196	20.501	29.248	1.00	52.89	C
ATOM	2362	CB	PHE	A	308	44.935	20.374	30.118	1.00	52.27	C
ATOM	2363	CG	PHE	A	308	44.417	18.951	30.224	1.00	51.21	C
ATOM	2364	CD1	PHE	A	308	43.367	18.501	29.427	1.00	50.32	C
ATOM	2365	CE1	PHE	A	308	42.882	17.174	29.523	1.00	48.18	C
ATOM	2366	CZ	PHE	A	308	43.453	16.290	30.396	1.00	46.18	C
ATOM	2367	CE2	PHE	A	308	44.504	16.709	31.178	1.00	48.53	C
ATOM	2368	CD2	PHE	A	308	44.990	18.042	31.092	1.00	50.45	C
ATOM	2369	C	PHE	A	308	46.353	21.889	28.555	1.00	53.68	C
ATOM	2370	O	PHE	A	308	46.035	22.045	27.374	1.00	53.62	O
ATOM	2371	N	LYS	A	309	46.870	22.878	29.276	1.00	54.73	N
ATOM	2372	CA	LYS	A	309	47.200	24.188	28.702	1.00	55.83	C
ATOM	2373	CB	LYS	A	309	47.708	25.144	29.800	1.00	56.03	C
ATOM	2374	CG	LYS	A	309	46.955	26.519	30.015	1.00	56.81	C
ATOM	2375	CD	LYS	A	309	45.381	26.496	30.075	1.00	56.75	C
ATOM	2376	CE	LYS	A	309	44.748	27.808	29.452	1.00	56.68	C
ATOM	2377	NZ	LYS	A	309	43.870	28.707	30.322	1.00	54.22	N
ATOM	2378	C	LYS	A	309	48.243	24.043	27.587	1.00	56.34	C
ATOM	2379	O	LYS	A	309	48.111	24.622	26.519	1.00	56.10	O
ATOM	2380	N	GLU	A	310	49.264	23.238	27.827	1.00	57.67	N
ATOM	2381	CA	GLU	A	310	50.261	22.930	26.794	1.00	59.38	C
ATOM	2382	CB	GLU	A	310	51.426	22.152	27.428	1.00	59.22	C
ATOM	2383	CG	GLU	A	310	52.749	22.241	26.665	1.00	60.98	C
ATOM	2384	CD	GLU	A	310	53.627	23.470	26.978	1.00	62.34	C
ATOM	2385	OE1	GLU	A	310	53.415	24.193	27.996	1.00	62.42	O
ATOM	2386	OE2	GLU	A	310	54.567	23.705	26.181	1.00	62.23	O
ATOM	2387	C	GLU	A	310	49.691	22.163	25.561	1.00	60.15	C
ATOM	2388	O	GLU	A	310	50.189	22.284	24.419	1.00	59.92	O
ATOM	2389	N	ALA	A	311	48.651	21.363	25.808	1.00	61.12	N
ATOM	2390	CA	ALA	A	311	48.102	20.475	24.780	1.00	61.40	C
ATOM	2391	CB	ALA	A	311	47.399	19.261	25.407	1.00	61.19	C
ATOM	2392	C	ALA	A	311	47.147	21.275	23.940	1.00	61.58	C
ATOM	2393	O	ALA	A	311	47.251	21.265	22.709	1.00	61.80	O
ATOM	2394	N	GLU	A	312	46.240	21.986	24.622	1.00	61.49	N
ATOM	2395	CA	GLU	A	312	45.275	22.850	23.973	1.00	61.47	C
ATOM	2396	CB	GLU	A	312	44.395	23.532	25.017	1.00	61.25	C
ATOM	2397	CG	GLU	A	312	43.800	24.871	24.619	1.00	62.27	C
ATOM	2398	CD	GLU	A	312	44.147	25.972	25.615	1.00	63.79	C
ATOM	2399	OE1	GLU	A	312	45.356	26.270	25.756	1.00	65.56	O
ATOM	2400	OE2	GLU	A	312	43.228	26.542	26.260	1.00	63.29	O
ATOM	2401	C	GLU	A	312	46.037	23.823	23.079	1.00	61.57	C
ATOM	2402	O	GLU	A	312	45.587	24.147	21.982	1.00	61.69	O
ATOM	2403	N	LYS	A	313	47.228	24.234	23.512	1.00	61.82	N
ATOM	2404	CA	LYS	A	313	48.118	25.014	22.633	1.00	62.05	C
ATOM	2405	CB	LYS	A	313	49.463	25.338	23.325	1.00	62.73	C

244/396

Figure 3A-44

ATOM	2406	CG	LYS	A	313	50.736	25.121	22.433	1.00	64.78	C
ATOM	2407	CD	LYS	A	313	51.508	26.423	22.130	1.00	67.36	C
ATOM	2408	CE	LYS	A	313	51.497	26.769	20.631	1.00	68.72	C
ATOM	2409	NZ	LYS	A	313	50.258	27.524	20.195	1.00	69.59	N
ATOM	2410	C	LYS	A	313	48.361	24.326	21.275	1.00	61.00	C
ATOM	2411	O	LYS	A	313	48.172	24.928	20.217	1.00	60.72	O
ATOM	2412	N	PHE	A	314	48.769	23.064	21.327	1.00	59.95	N
ATOM	2413	CA	PHE	A	314	49.126	22.339	20.136	1.00	59.05	C
ATOM	2414	CB	PHE	A	314	49.394	20.884	20.482	1.00	59.12	C
ATOM	2415	CG	PHE	A	314	50.044	20.084	19.373	1.00	59.39	C
ATOM	2416	CD1	PHE	A	314	51.053	19.177	19.664	1.00	59.54	C
ATOM	2417	CE1	PHE	A	314	51.642	18.408	18.675	1.00	59.75	C
ATOM	2418	CZ	PHE	A	314	51.224	18.524	17.377	1.00	61.24	C
ATOM	2419	CE2	PHE	A	314	50.208	19.416	17.064	1.00	62.30	C
ATOM	2420	CD2	PHE	A	314	49.617	20.183	18.065	1.00	60.44	C
ATOM	2421	C	PHE	A	314	48.056	22.471	19.056	1.00	58.49	C
ATOM	2422	O	PHE	A	314	48.402	22.543	17.888	1.00	58.87	O
ATOM	2423	N	PHE	A	315	46.774	22.520	19.410	1.00	57.45	N
ATOM	2424	CA	PHE	A	315	45.760	22.686	18.368	1.00	56.48	C
ATOM	2425	CB	PHE	A	315	44.356	22.463	18.881	1.00	56.22	C
ATOM	2426	CG	PHE	A	315	44.046	21.065	19.138	1.00	54.82	C
ATOM	2427	CD1	PHE	A	315	44.083	20.143	18.104	1.00	52.68	C
ATOM	2428	CE1	PHE	A	315	43.791	18.823	18.354	1.00	53.36	C
ATOM	2429	CZ	PHE	A	315	43.460	18.408	19.661	1.00	53.35	C
ATOM	2430	CE2	PHE	A	315	43.434	19.330	20.703	1.00	53.27	C
ATOM	2431	CD2	PHE	A	315	43.722	20.652	20.434	1.00	54.04	C
ATOM	2432	C	PHE	A	315	45.813	24.072	17.830	1.00	56.43	C
ATOM	2433	O	PHE	A	315	45.937	24.268	16.634	1.00	56.05	O
ATOM	2434	N	VAL	A	316	45.715	25.043	18.722	1.00	56.65	N
ATOM	2435	CA	VAL	A	316	45.620	26.405	18.268	1.00	57.63	C
ATOM	2436	CB	VAL	A	316	45.158	27.341	19.388	1.00	57.60	C
ATOM	2437	CG1	VAL	A	316	46.344	27.845	20.222	1.00	58.63	C
ATOM	2438	CG2	VAL	A	316	44.298	28.497	18.789	1.00	58.13	C
ATOM	2439	C	VAL	A	316	46.901	26.849	17.531	1.00	58.16	C
ATOM	2440	O	VAL	A	316	46.881	27.795	16.733	1.00	58.10	O
ATOM	2441	N	SER	A	317	47.992	26.125	17.787	1.00	58.90	N
ATOM	2442	CA	SER	A	317	49.217	26.168	16.973	1.00	59.44	C
ATOM	2443	CB	SER	A	317	50.258	25.191	17.533	1.00	59.66	C
ATOM	2444	OG	SER	A	317	50.651	24.238	16.555	1.00	59.27	O
ATOM	2445	C	SER	A	317	48.992	25.850	15.481	1.00	59.64	C
ATOM	2446	O	SER	A	317	49.729	26.349	14.616	1.00	59.47	O
ATOM	2447	N	VAL	A	318	47.997	25.008	15.202	1.00	59.65	N
ATOM	2448	CA	VAL	A	318	47.574	24.758	13.834	1.00	59.93	C
ATOM	2449	CB	VAL	A	318	47.790	23.303	13.416	1.00	59.75	C
ATOM	2450	CG1	VAL	A	318	49.175	23.137	12.930	1.00	59.50	C
ATOM	2451	CG2	VAL	A	318	47.530	22.357	14.570	1.00	60.07	C
ATOM	2452	C	VAL	A	318	46.133	25.192	13.533	1.00	60.34	C
ATOM	2453	O	VAL	A	318	45.476	24.595	12.689	1.00	60.59	O
ATOM	2454	N	GLY	A	319	45.641	26.229	14.202	1.00	60.67	N
ATOM	2455	CA	GLY	A	319	44.337	26.768	13.852	1.00	61.49	C
ATOM	2456	C	GLY	A	319	43.190	26.444	14.796	1.00	62.03	C
ATOM	2457	O	GLY	A	319	42.543	27.351	15.322	1.00	62.52	O
ATOM	2458	N	LEU	A	320	42.934	25.162	15.022	1.00	62.32	N
ATOM	2459	CA	LEU	A	320	41.822	24.739	15.875	1.00	62.86	C
ATOM	2460	CB	LEU	A	320	41.881	23.223	16.070	1.00	62.82	C
ATOM	2461	CG	LEU	A	320	41.279	22.343	14.975	1.00	62.36	C

245/396

Figure 3A-45

ATOM	2462	CD1	LEU	A	320	39.922	22.823	14.460	1.00	61.51	C
ATOM	2463	CD2	LEU	A	320	42.271	22.229	13.844	1.00	62.90	C
ATOM	2464	C	LEU	A	320	41.680	25.481	17.236	1.00	63.42	C
ATOM	2465	O	LEU	A	320	42.640	25.571	17.998	1.00	63.27	O
ATOM	2466	N	PRO	A	321	40.463	25.948	17.546	1.00	64.13	N
ATOM	2467	CA	PRO	A	321	40.215	26.969	18.586	1.00	64.57	C
ATOM	2468	CB	PRO	A	321	38.676	26.944	18.731	1.00	64.76	C
ATOM	2469	CG	PRO	A	321	38.202	25.664	18.045	1.00	63.98	C
ATOM	2470	CD	PRO	A	321	39.194	25.481	16.942	1.00	64.23	C
ATOM	2471	C	PRO	A	321	40.850	26.771	19.978	1.00	65.09	C
ATOM	2472	O	PRO	A	321	41.291	25.656	20.312	1.00	64.89	O
ATOM	2473	N	ASN	A	322	40.889	27.865	20.755	1.00	65.76	N
ATOM	2474	CA	ASN	A	322	41.248	27.861	22.184	1.00	66.80	C
ATOM	2475	CB	ASN	A	322	41.350	29.309	22.756	1.00	67.27	C
ATOM	2476	CG	ASN	A	322	42.689	30.050	22.423	1.00	68.08	C
ATOM	2477	OD1	ASN	A	322	43.777	29.683	22.905	1.00	68.98	O
ATOM	2478	ND2	ASN	A	322	42.578	31.149	21.660	1.00	67.50	N
ATOM	2479	C	ASN	A	322	40.100	27.129	22.909	1.00	67.24	C
ATOM	2480	O	ASN	A	322	38.926	27.274	22.497	1.00	67.55	O
ATOM	2481	N	MET	A	323	40.398	26.379	23.976	1.00	67.41	N
ATOM	2482	CA	MET	A	323	39.350	25.619	24.682	1.00	67.61	C
ATOM	2483	CB	MET	A	323	39.958	24.583	25.617	1.00	67.65	C
ATOM	2484	CG	MET	A	323	40.487	23.350	24.923	1.00	67.06	C
ATOM	2485	SD	MET	A	323	39.506	21.872	25.237	1.00	66.23	S
ATOM	2486	CE	MET	A	323	39.518	21.220	23.599	1.00	64.93	C
ATOM	2487	C	MET	A	323	38.459	26.547	25.475	1.00	68.02	C
ATOM	2488	O	MET	A	323	38.964	27.510	26.051	1.00	67.91	O
ATOM	2489	N	THR	A	324	37.156	26.239	25.521	1.00	68.79	N
ATOM	2490	CA	THR	A	324	36.104	27.138	26.084	1.00	69.68	C
ATOM	2491	CB	THR	A	324	34.634	26.571	25.818	1.00	69.62	C
ATOM	2492	OG1	THR	A	324	34.241	25.645	26.846	1.00	69.29	O
ATOM	2493	CG2	THR	A	324	34.563	25.719	24.569	1.00	69.98	C
ATOM	2494	C	THR	A	324	36.241	27.490	27.585	1.00	70.09	C
ATOM	2495	O	THR	A	324	36.477	26.596	28.392	1.00	70.76	O
ATOM	2496	N	GLN	A	325	36.093	28.762	27.969	1.00	70.02	N
ATOM	2497	CA	GLN	A	325	35.848	29.073	29.382	1.00	70.36	C
ATOM	2498	CB	GLN	A	325	35.795	30.601	29.638	1.00	70.60	C
ATOM	2499	CG	GLN	A	325	35.988	31.093	31.098	1.00	72.10	C
ATOM	2500	CD	GLN	A	325	35.014	30.439	32.121	1.00	76.60	C
ATOM	2501	OE1	GLN	A	325	33.979	31.024	32.484	1.00	77.84	O
ATOM	2502	NE2	GLN	A	325	35.353	29.228	32.582	1.00	77.39	N
ATOM	2503	C	GLN	A	325	34.497	28.396	29.667	1.00	70.35	C
ATOM	2504	O	GLN	A	325	33.467	28.815	29.141	1.00	70.56	O
ATOM	2505	N	GLY	A	326	34.489	27.340	30.470	1.00	70.30	N
ATOM	2506	CA	GLY	A	326	33.282	26.543	30.615	1.00	70.39	C
ATOM	2507	C	GLY	A	326	33.578	25.082	30.359	1.00	70.58	C
ATOM	2508	O	GLY	A	326	32.889	24.206	30.881	1.00	70.41	O
ATOM	2509	N	PHE	A	327	34.577	24.839	29.506	1.00	70.99	N
ATOM	2510	CA	PHE	A	327	35.383	23.615	29.535	1.00	71.22	C
ATOM	2511	CB	PHE	A	327	36.332	23.532	28.335	1.00	71.52	C
ATOM	2512	CG	PHE	A	327	37.432	22.471	28.466	1.00	72.91	C
ATOM	2513	CD1	PHE	A	327	38.648	22.764	29.070	1.00	72.49	C
ATOM	2514	CE1	PHE	A	327	39.644	21.809	29.157	1.00	72.46	C
ATOM	2515	CZ	PHE	A	327	39.452	20.541	28.626	1.00	73.83	C
ATOM	2516	CE2	PHE	A	327	38.263	20.219	28.003	1.00	74.32	C
ATOM	2517	CD2	PHE	A	327	37.257	21.186	27.920	1.00	75.37	C

246/396

Figure 3A-46

ATOM	2518	C	PHE	A	327	36.216	23.630	30.798	1.00	70.95	C
ATOM	2519	O	PHE	A	327	36.084	22.718	31.606	1.00	71.18	O
ATOM	2520	N	TRP	A	328	37.058	24.666	30.963	1.00	70.53	N
ATOM	2521	CA	TRP	A	328	37.982	24.742	32.096	1.00	70.28	C
ATOM	2522	CB	TRP	A	328	38.964	25.936	32.055	1.00	70.88	C
ATOM	2523	CG	TRP	A	328	39.918	26.018	30.889	1.00	72.09	C
ATOM	2524	CD1	TRP	A	328	39.974	27.024	29.977	1.00	73.68	C
ATOM	2525	NE1	TRP	A	328	40.952	26.765	29.048	1.00	75.20	N
ATOM	2526	CE2	TRP	A	328	41.566	25.581	29.356	1.00	73.79	C
ATOM	2527	CD2	TRP	A	328	40.954	25.087	30.520	1.00	72.89	C
ATOM	2528	CE3	TRP	A	328	41.404	23.870	31.034	1.00	74.11	C
ATOM	2529	CZ3	TRP	A	328	42.447	23.197	30.376	1.00	74.50	C
ATOM	2530	CH2	TRP	A	328	43.039	23.728	29.233	1.00	74.15	C
ATOM	2531	CZ2	TRP	A	328	42.614	24.912	28.707	1.00	73.94	C
ATOM	2532	C	TRP	A	328	37.214	24.803	33.394	1.00	69.71	C
ATOM	2533	O	TRP	A	328	37.669	24.236	34.397	1.00	69.91	O
ATOM	2534	N	GLU	A	329	36.059	25.474	33.375	1.00	68.71	N
ATOM	2535	CA	GLU	A	329	35.288	25.709	34.600	1.00	68.04	C
ATOM	2536	CB	GLU	A	329	34.189	26.770	34.366	1.00	68.47	C
ATOM	2537	CG	GLU	A	329	33.301	27.116	35.572	1.00	70.17	C
ATOM	2538	CD	GLU	A	329	33.699	28.403	36.296	1.00	72.62	C
ATOM	2539	OE1	GLU	A	329	33.991	29.424	35.623	1.00	74.84	O
ATOM	2540	OE2	GLU	A	329	33.706	28.405	37.549	1.00	72.70	O
ATOM	2541	C	GLU	A	329	34.742	24.437	35.287	1.00	67.01	C
ATOM	2542	O	GLU	A	329	34.729	24.356	36.524	1.00	67.20	O
ATOM	2543	N	ASN	A	330	34.318	23.434	34.525	1.00	65.45	N
ATOM	2544	CA	ASN	A	330	33.745	22.270	35.177	1.00	64.30	C
ATOM	2545	CB	ASN	A	330	32.252	22.430	35.301	1.00	64.41	C
ATOM	2546	CG	ASN	A	330	31.618	22.672	33.973	1.00	65.81	C
ATOM	2547	OD1	ASN	A	330	31.045	21.766	33.379	1.00	66.48	O
ATOM	2548	ND2	ASN	A	330	31.747	23.896	33.465	1.00	67.91	N
ATOM	2549	C	ASN	A	330	34.086	20.953	34.525	1.00	63.39	C
ATOM	2550	O	ASN	A	330	33.409	19.952	34.762	1.00	63.58	O
ATOM	2551	N	SER	A	331	35.147	20.944	33.726	1.00	62.30	N
ATOM	2552	CA	SER	A	331	35.846	19.696	33.405	1.00	61.65	C
ATOM	2553	CB	SER	A	331	36.672	19.837	32.140	1.00	61.53	C
ATOM	2554	OG	SER	A	331	37.104	18.560	31.725	1.00	61.69	O
ATOM	2555	C	SER	A	331	36.763	19.254	34.550	1.00	61.32	C
ATOM	2556	O	SER	A	331	37.275	20.087	35.302	1.00	61.40	O
ATOM	2557	N	MET	A	332	36.996	17.949	34.654	1.00	60.84	N
ATOM	2558	CA	MET	A	332	37.646	17.363	35.827	1.00	60.63	C
ATOM	2559	CB	MET	A	332	36.626	16.526	36.610	1.00	60.03	C
ATOM	2560	CG	MET	A	332	37.211	15.374	37.404	1.00	58.21	C
ATOM	2561	SD	MET	A	332	36.333	15.033	38.906	1.00	55.80	S
ATOM	2562	CE	MET	A	332	36.727	16.522	39.826	1.00	56.67	C
ATOM	2563	C	MET	A	332	38.891	16.528	35.505	1.00	61.40	C
ATOM	2564	O	MET	A	332	38.823	15.296	35.457	1.00	61.48	O
ATOM	2565	N	LEU	A	333	40.030	17.193	35.316	1.00	62.37	N
ATOM	2566	CA	LEU	A	333	41.300	16.516	34.954	1.00	63.35	C
ATOM	2567	CB	LEU	A	333	42.021	17.287	33.843	1.00	62.69	C
ATOM	2568	CG	LEU	A	333	41.160	18.429	33.323	1.00	61.75	C
ATOM	2569	CD1	LEU	A	333	41.495	19.695	34.084	1.00	62.76	C
ATOM	2570	CD2	LEU	A	333	41.321	18.628	31.861	1.00	59.82	C
ATOM	2571	C	LEU	A	333	42.238	16.227	36.155	1.00	64.47	C
ATOM	2572	O	LEU	A	333	43.459	16.096	36.010	1.00	64.47	O
ATOM	2573	N	THR	A	334	41.625	16.141	37.334	1.00	65.81	N

247/396

Figure 3A-47

ATOM	2574	CA	THR	A	334	42.257	15.734	38.577	1.00	67.03	C
ATOM	2575	CB	THR	A	334	42.195	16.904	39.625	1.00	66.83	C
ATOM	2576	OG1	THR	A	334	40.835	17.272	39.862	1.00	67.28	O
ATOM	2577	CG2	THR	A	334	42.770	18.225	39.075	1.00	66.51	C
ATOM	2578	C	THR	A	334	41.403	14.546	39.057	1.00	68.23	C
ATOM	2579	O	THR	A	334	40.210	14.472	38.719	1.00	68.64	O
ATOM	2580	N	ASP	A	335	41.975	13.605	39.810	1.00	69.28	N
ATOM	2581	CA	ASP	A	335	41.115	12.832	40.700	1.00	69.83	C
ATOM	2582	CB	ASP	A	335	41.567	11.408	41.035	1.00	70.06	C
ATOM	2583	CG	ASP	A	335	40.429	10.567	41.703	1.00	71.10	C
ATOM	2584	OD1	ASP	A	335	40.502	9.308	41.734	1.00	71.35	O
ATOM	2585	OD2	ASP	A	335	39.401	11.079	42.214	1.00	72.04	O
ATOM	2586	C	ASP	A	335	41.113	13.626	41.946	1.00	70.11	C
ATOM	2587	O	ASP	A	335	42.165	13.917	42.499	1.00	69.98	O
ATOM	2588	N	PRO	A	336	39.915	14.025	42.335	1.00	70.84	N
ATOM	2589	CA	PRO	A	336	39.616	14.526	43.686	1.00	71.58	C
ATOM	2590	CB	PRO	A	336	38.136	14.882	43.575	1.00	71.49	C
ATOM	2591	CG	PRO	A	336	37.646	13.967	42.454	1.00	71.14	C
ATOM	2592	CD	PRO	A	336	38.733	14.043	41.457	1.00	70.62	C
ATOM	2593	C	PRO	A	336	39.864	13.461	44.811	1.00	72.15	C
ATOM	2594	O	PRO	A	336	39.903	13.810	46.012	1.00	71.90	O
ATOM	2595	N	GLY	A	337	40.006	12.190	44.407	1.00	72.71	N
ATOM	2596	CA	GLY	A	337	40.538	11.116	45.247	1.00	73.38	C
ATOM	2597	C	GLY	A	337	39.551	10.348	46.110	1.00	73.80	C
ATOM	2598	O	GLY	A	337	38.660	9.636	45.592	1.00	73.85	O
ATOM	2599	N	ASN	A	338	39.747	10.475	47.429	1.00	73.95	N
ATOM	2600	CA	ASN	A	338	38.821	9.951	48.436	1.00	74.09	C
ATOM	2601	CB	ASN	A	338	39.579	9.559	49.716	1.00	74.10	C
ATOM	2602	CG	ASN	A	338	40.105	8.110	49.691	1.00	74.57	C
ATOM	2603	OD1	ASN	A	338	39.362	7.138	49.912	1.00	74.83	O
ATOM	2604	ND2	ASN	A	338	41.399	7.970	49.448	1.00	75.38	N
ATOM	2605	C	ASN	A	338	37.715	10.985	48.725	1.00	74.06	C
ATOM	2606	O	ASN	A	338	37.857	12.162	48.355	1.00	74.17	O
ATOM	2607	N	VAL	A	339	36.639	10.547	49.390	1.00	73.86	N
ATOM	2608	CA	VAL	A	339	35.372	11.300	49.539	1.00	73.91	C
ATOM	2609	CB	VAL	A	339	35.436	12.731	50.285	1.00	74.13	C
ATOM	2610	CG1	VAL	A	339	35.121	12.641	51.797	1.00	74.37	C
ATOM	2611	CG2	VAL	A	339	36.698	13.574	49.960	1.00	73.72	C
ATOM	2612	C	VAL	A	339	34.628	11.531	48.220	1.00	73.84	C
ATOM	2613	O	VAL	A	339	33.553	12.164	48.240	1.00	74.58	O
ATOM	2614	N	GLN	A	340	35.181	11.049	47.092	1.00	72.81	N
ATOM	2615	CA	GLN	A	340	34.596	11.293	45.753	1.00	71.24	C
ATOM	2616	CB	GLN	A	340	34.813	12.748	45.315	1.00	71.34	C
ATOM	2617	CG	GLN	A	340	33.553	13.492	44.925	1.00	72.26	C
ATOM	2618	CD	GLN	A	340	33.703	14.236	43.595	1.00	74.84	C
ATOM	2619	OE1	GLN	A	340	33.896	13.595	42.559	1.00	74.85	O
ATOM	2620	NE2	GLN	A	340	33.626	15.589	43.622	1.00	75.26	N
ATOM	2621	C	GLN	A	340	35.098	10.303	44.691	1.00	69.94	C
ATOM	2622	O	GLN	A	340	35.848	10.660	43.769	1.00	70.00	O
ATOM	2623	N	LYS	A	341	34.665	9.054	44.848	1.00	68.21	N
ATOM	2624	CA	LYS	A	341	34.918	7.958	43.905	1.00	66.57	C
ATOM	2625	CB	LYS	A	341	34.500	6.623	44.540	1.00	66.28	C
ATOM	2626	CG	LYS	A	341	33.140	6.615	45.271	1.00	65.44	C
ATOM	2627	CD	LYS	A	341	32.857	7.874	46.128	1.00	63.50	C
ATOM	2628	CE	LYS	A	341	33.154	7.661	47.603	1.00	62.15	C
ATOM	2629	NZ	LYS	A	341	32.966	6.245	48.018	1.00	60.94	N

248/396

Figure 3A-48

ATOM	2630	C	LYS	A	341	34.225	8.170	42.537	1.00	65.56	C
ATOM	2631	O	LYS	A	341	33.008	8.361	42.487	1.00	65.67	O
ATOM	2632	N	ALA	A	342	34.999	8.095	41.446	1.00	64.04	N
ATOM	2633	CA	ALA	A	342	34.611	8.647	40.153	1.00	62.76	C
ATOM	2634	CB	ALA	A	342	34.998	10.122	40.142	1.00	62.96	C
ATOM	2635	C	ALA	A	342	35.252	7.967	38.937	1.00	62.03	C
ATOM	2636	O	ALA	A	342	36.412	8.264	38.651	1.00	62.16	O
ATOM	2637	N	VAL	A	343	34.507	7.132	38.190	1.00	60.90	N
ATOM	2638	CA	VAL	A	343	35.051	6.393	37.014	1.00	59.90	C
ATOM	2639	CB	VAL	A	343	34.014	6.063	35.855	1.00	59.80	C
ATOM	2640	CG1	VAL	A	343	33.298	4.754	36.068	1.00	59.72	C
ATOM	2641	CG2	VAL	A	343	33.031	7.157	35.635	1.00	59.30	C
ATOM	2642	C	VAL	A	343	36.230	7.123	36.372	1.00	59.50	C
ATOM	2643	O	VAL	A	343	36.106	8.306	35.978	1.00	59.53	O
ATOM	2644	N	CYS	A	344	37.362	6.421	36.249	1.00	58.48	N
ATOM	2645	CA	CYS	A	344	38.623	7.119	35.969	1.00	57.55	C
ATOM	2646	CB	CYS	A	344	39.714	6.721	36.947	1.00	57.12	C
ATOM	2647	SG	CYS	A	344	39.717	7.905	38.282	1.00	58.61	S
ATOM	2648	C	CYS	A	344	39.196	7.197	34.557	1.00	56.67	C
ATOM	2649	O	CYS	A	344	38.789	6.433	33.648	1.00	55.70	O
ATOM	2650	N	HIS	A	345	40.233	8.433	34.480	1.00	25.00	AN
ATOM	2651	CA	HIS	A	345	41.288	8.513	33.471	1.00	25.00	AC
ATOM	2652	C	HIS	A	345	40.852	8.654	31.993	1.00	25.00	AC
ATOM	2653	O	HIS	A	345	41.396	9.465	31.230	1.00	25.00	AO
ATOM	2654	CB	HIS	A	345	42.215	7.291	33.634	1.00	25.00	AC
ATOM	2655	CG	HIS	A	345	43.673	7.623	33.556	1.00	25.00	AC
ATOM	2656	ND1	HIS	A	345	44.217	8.735	34.165	1.00	25.00	AN
ATOM	2657	CD2	HIS	A	345	44.696	7.000	32.925	1.00	25.00	AC
ATOM	2658	CE1	HIS	A	345	45.514	8.778	33.920	1.00	25.00	AC
ATOM	2659	NE2	HIS	A	345	45.830	7.737	33.169	1.00	25.00	AN
ATOM	2660	N	PRO	A	346	39.811	7.583	31.413	1.00	51.61	N
ATOM	2661	CA	PRO	A	346	39.597	7.475	29.982	1.00	51.37	C
ATOM	2662	CB	PRO	A	346	38.922	6.081	29.845	1.00	51.43	C
ATOM	2663	CG	PRO	A	346	38.945	5.452	31.289	1.00	50.06	C
ATOM	2664	CD	PRO	A	346	38.930	6.645	32.143	1.00	50.68	C
ATOM	2665	C	PRO	A	346	38.809	8.616	29.269	1.00	51.11	C
ATOM	2666	O	PRO	A	346	39.171	8.848	28.112	1.00	51.41	O
ATOM	2667	N	THR	A	347	37.832	9.297	29.887	1.00	50.18	N
ATOM	2668	CA	THR	A	347	36.683	9.807	29.094	1.00	49.83	C
ATOM	2669	CB	THR	A	347	35.324	9.360	29.692	1.00	49.81	C
ATOM	2670	OG1	THR	A	347	34.652	10.518	30.188	1.00	50.80	O
ATOM	2671	CG2	THR	A	347	35.461	8.452	30.947	1.00	49.64	C
ATOM	2672	C	THR	A	347	36.604	11.290	28.663	1.00	49.60	C
ATOM	2673	O	THR	A	347	37.244	12.130	29.266	1.00	50.08	O
ATOM	2674	N	ALA	A	348	35.776	11.589	27.643	1.00	49.56	N
ATOM	2675	CA	ALA	A	348	35.698	12.913	26.949	1.00	49.40	C
ATOM	2676	CB	ALA	A	348	36.598	12.864	25.754	1.00	49.69	C
ATOM	2677	C	ALA	A	348	34.273	13.397	26.498	1.00	49.17	C
ATOM	2678	O	ALA	A	348	33.690	12.836	25.558	1.00	49.33	O
ATOM	2679	N	TRP	A	349	33.726	14.441	27.130	1.00	48.67	N
ATOM	2680	CA	TRP	A	349	32.259	14.667	27.086	1.00	48.13	C
ATOM	2681	CB	TRP	A	349	31.653	14.820	28.499	1.00	47.14	C
ATOM	2682	CG	TRP	A	349	31.839	13.615	29.389	1.00	44.86	C
ATOM	2683	CD1	TRP	A	349	32.989	12.919	29.583	1.00	42.74	C
ATOM	2684	NE1	TRP	A	349	32.789	11.873	30.448	1.00	39.87	N
ATOM	2685	CE2	TRP	A	349	31.487	11.875	30.855	1.00	41.57	C

249/396

Figure 3A-49

ATOM	2686	CD2	TRP	A	349	30.850	12.970	30.210	1.00	44.02	C
ATOM	2687	CE3	TRP	A	349	29.479	13.190	30.460	1.00	44.69	C
ATOM	2688	CZ3	TRP	A	349	28.808	12.316	31.349	1.00	43.52	C
ATOM	2689	CH2	TRP	A	349	29.487	11.234	31.962	1.00	41.02	C
ATOM	2690	CZ2	TRP	A	349	30.811	10.998	31.724	1.00	40.50	C
ATOM	2691	C	TRP	A	349	31.734	15.773	26.147	1.00	49.03	C
ATOM	2692	O	TRP	A	349	32.259	16.919	26.082	1.00	48.93	O
ATOM	2693	N	ASP	A	350	30.701	15.387	25.396	1.00	49.60	N
ATOM	2694	CA	ASP	A	350	29.865	16.322	24.647	1.00	50.25	C
ATOM	2695	CB	ASP	A	350	29.803	15.931	23.149	1.00	50.32	C
ATOM	2696	CG	ASP	A	350	28.995	16.933	22.263	1.00	50.86	C
ATOM	2697	OD1	ASP	A	350	28.862	16.677	21.033	1.00	51.65	O
ATOM	2698	OD2	ASP	A	350	28.460	17.987	22.686	1.00	51.88	O
ATOM	2699	C	ASP	A	350	28.508	16.188	25.326	1.00	50.23	C
ATOM	2700	O	ASP	A	350	27.714	15.329	24.953	1.00	50.59	O
ATOM	2701	N	LEU	A	351	28.247	16.984	26.358	1.00	49.94	N
ATOM	2702	CA	LEU	A	351	26.994	16.785	27.066	1.00	49.99	C
ATOM	2703	CB	LEU	A	351	26.997	17.396	28.464	1.00	49.28	C
ATOM	2704	CG	LEU	A	351	28.249	17.160	29.283	1.00	47.02	C
ATOM	2705	CD1	LEU	A	351	29.092	18.384	29.184	1.00	44.43	C
ATOM	2706	CD2	LEU	A	351	27.896	16.880	30.690	1.00	44.75	C
ATOM	2707	C	LEU	A	351	25.888	17.357	26.213	1.00	51.07	C
ATOM	2708	O	LEU	A	351	24.728	16.989	26.368	1.00	51.57	O
ATOM	2709	N	GLY	A	352	26.261	18.230	25.284	1.00	51.93	N
ATOM	2710	CA	GLY	A	352	25.300	18.846	24.391	1.00	53.52	C
ATOM	2711	C	GLY	A	352	25.168	20.306	24.715	1.00	54.86	C
ATOM	2712	O	GLY	A	352	25.840	20.798	25.618	1.00	55.38	O
ATOM	2713	N	LYS	A	353	24.311	21.011	23.985	1.00	56.04	N
ATOM	2714	CA	LYS	A	353	24.127	22.451	24.196	1.00	57.18	C
ATOM	2715	CB	LYS	A	353	23.278	22.740	25.442	1.00	57.39	C
ATOM	2716	CG	LYS	A	353	22.696	24.166	25.429	1.00	60.78	C
ATOM	2717	CD	LYS	A	353	22.199	24.633	23.989	1.00	64.36	C
ATOM	2718	CE	LYS	A	353	22.617	26.081	23.616	1.00	64.56	C
ATOM	2719	NZ	LYS	A	353	22.198	26.454	22.222	1.00	64.94	N
ATOM	2720	C	LYS	A	353	25.441	23.242	24.256	1.00	57.10	C
ATOM	2721	O	LYS	A	353	25.507	24.342	24.815	1.00	57.09	O
ATOM	2722	N	GLY	A	354	26.478	22.679	23.651	1.00	57.39	N
ATOM	2723	CA	GLY	A	354	27.774	23.312	23.635	1.00	57.27	C
ATOM	2724	C	GLY	A	354	28.289	23.321	25.037	1.00	57.32	C
ATOM	2725	O	GLY	A	354	28.722	24.341	25.526	1.00	57.33	O
ATOM	2726	N	ASP	A	355	28.194	22.182	25.698	1.00	57.76	N
ATOM	2727	CA	ASP	A	355	28.908	21.989	26.945	1.00	58.48	C
ATOM	2728	CB	ASP	A	355	27.956	21.773	28.117	1.00	58.71	C
ATOM	2729	CG	ASP	A	355	28.688	21.488	29.422	1.00	60.63	C
ATOM	2730	OD1	ASP	A	355	28.011	20.964	30.336	1.00	62.79	O
ATOM	2731	OD2	ASP	A	355	29.917	21.726	29.625	1.00	60.95	O
ATOM	2732	C	ASP	A	355	29.937	20.862	26.803	1.00	58.43	C
ATOM	2733	O	ASP	A	355	29.658	19.770	26.288	1.00	58.42	O
ATOM	2734	N	PHE	A	356	31.127	21.149	27.309	1.00	58.42	N
ATOM	2735	CA	PHE	A	356	32.335	20.458	26.891	1.00	58.10	C
ATOM	2736	CB	PHE	A	356	32.991	21.324	25.818	1.00	58.39	C
ATOM	2737	CG	PHE	A	356	32.510	21.044	24.419	1.00	58.74	C
ATOM	2738	CD1	PHE	A	356	32.651	22.011	23.422	1.00	58.78	C
ATOM	2739	CE1	PHE	A	356	32.243	21.755	22.106	1.00	58.45	C
ATOM	2740	CZ	PHE	A	356	31.697	20.531	21.776	1.00	58.56	C
ATOM	2741	CE2	PHE	A	356	31.570	19.543	22.758	1.00	60.39	C

250/396

Figure 3A-50

ATOM	2742	CD2	PHE	A	356	31.979	19.801	24.077	1.00	59.53	C
ATOM	2743	C	PHE	A	356	33.298	20.223	28.077	1.00	57.35	C
ATOM	2744	O	PHE	A	356	33.763	21.185	28.708	1.00	56.89	O
ATOM	2745	N	ARG	A	357	33.581	18.947	28.360	1.00	56.21	N
ATOM	2746	CA	ARG	A	357	34.225	18.529	29.600	1.00	55.47	C
ATOM	2747	CB	ARG	A	357	33.172	18.203	30.688	1.00	55.61	C
ATOM	2748	CG	ARG	A	357	32.198	19.319	31.186	1.00	57.89	C
ATOM	2749	CD	ARG	A	357	30.834	18.780	31.765	1.00	61.07	C
ATOM	2750	NE	ARG	A	357	30.335	19.396	33.010	1.00	61.71	N
ATOM	2751	CZ	ARG	A	357	29.053	19.703	33.261	1.00	61.27	C
ATOM	2752	NH1	ARG	A	357	28.717	20.248	34.425	1.00	61.31	N
ATOM	2753	NH2	ARG	A	357	28.106	19.473	32.358	1.00	60.75	N
ATOM	2754	C	ARG	A	357	35.016	17.251	29.373	1.00	54.58	C
ATOM	2755	O	ARG	A	357	34.430	16.255	28.960	1.00	54.94	O
ATOM	2756	N	ILE	A	358	36.320	17.245	29.661	1.00	53.24	N
ATOM	2757	CA	ILE	A	358	37.073	15.981	29.709	1.00	51.51	C
ATOM	2758	CB	ILE	A	358	38.519	16.177	29.276	1.00	51.10	C
ATOM	2759	CG1	ILE	A	358	38.587	16.583	27.811	1.00	50.56	C
ATOM	2760	CD1	ILE	A	358	39.844	16.152	27.131	1.00	49.52	C
ATOM	2761	CG2	ILE	A	358	39.301	14.910	29.543	1.00	49.59	C
ATOM	2762	C	ILE	A	358	37.121	15.495	31.121	1.00	50.91	C
ATOM	2763	O	ILE	A	358	37.666	16.189	31.947	1.00	50.66	O
ATOM	2764	N	LEU	A	359	36.589	14.318	31.412	1.00	50.44	N
ATOM	2765	CA	LEU	A	359	36.859	13.717	32.713	1.00	50.85	C
ATOM	2766	CB	LEU	A	359	35.671	12.916	33.193	1.00	49.92	C
ATOM	2767	CG	LEU	A	359	35.889	11.977	34.370	1.00	48.54	C
ATOM	2768	CD1	LEU	A	359	34.983	12.417	35.471	1.00	46.96	C
ATOM	2769	CD2	LEU	A	359	35.629	10.503	34.009	1.00	47.12	C
ATOM	2770	C	LEU	A	359	38.098	12.830	32.665	1.00	52.16	C
ATOM	2771	O	LEU	A	359	38.093	11.812	31.990	1.00	52.59	O
ATOM	2772	N	MET	A	360	39.162	13.203	33.374	1.00	53.87	N
ATOM	2773	CA	MET	A	360	40.397	12.378	33.410	1.00	55.68	C
ATOM	2774	CB	MET	A	360	41.329	12.734	32.237	1.00	55.70	C
ATOM	2775	CG	MET	A	360	42.675	11.985	32.154	1.00	55.51	C
ATOM	2776	SD	MET	A	360	43.584	12.546	30.661	1.00	56.78	S
ATOM	2777	CE	MET	A	360	45.101	11.819	30.892	1.00	56.16	C
ATOM	2778	C	MET	A	360	41.164	12.419	34.747	1.00	56.75	C
ATOM	2779	O	MET	A	360	41.230	13.467	35.417	1.00	56.65	O
ATOM	2780	N	CYS	A	361	41.742	11.277	35.130	1.00	57.76	N
ATOM	2781	CA	CYS	A	361	42.453	11.200	36.406	1.00	59.08	C
ATOM	2782	CB	CYS	A	361	42.173	9.853	37.103	1.00	59.07	C
ATOM	2783	SG	CYS	A	361	40.491	9.761	37.813	1.00	60.77	S
ATOM	2784	C	CYS	A	361	43.942	11.484	36.172	1.00	59.48	C
ATOM	2785	O	CYS	A	361	44.825	10.730	36.590	1.00	59.86	O
ATOM	2786	N	THR	A	362	44.202	12.600	35.496	1.00	60.05	N
ATOM	2787	CA	THR	A	362	45.531	12.900	34.963	1.00	60.50	C
ATOM	2788	CB	THR	A	362	45.604	14.298	34.321	1.00	60.49	C
ATOM	2789	OG1	THR	A	362	44.454	14.506	33.497	1.00	61.68	O
ATOM	2790	CG2	THR	A	362	46.774	14.375	33.336	1.00	60.19	C
ATOM	2791	C	THR	A	362	46.595	12.819	36.014	1.00	60.59	C
ATOM	2792	O	THR	A	362	46.488	13.450	37.076	1.00	61.03	O
ATOM	2793	N	LYS	A	363	47.611	12.023	35.696	1.00	60.48	N
ATOM	2794	CA	LYS	A	363	48.879	12.028	36.409	1.00	60.04	C
ATOM	2795	CB	LYS	A	363	49.222	10.604	36.895	1.00	60.04	C
ATOM	2796	CG	LYS	A	363	48.020	9.817	37.506	1.00	60.09	C
ATOM	2797	CD	LYS	A	363	47.637	8.522	36.712	1.00	59.47	C

251/396

Figure 3A-51

ATOM	2798	CE	LYS	A	363	47.868	7.207	37.535	1.00	57.86	C
ATOM	2799	NZ	LYS	A	363	48.681	6.126	36.857	1.00	55.17	N
ATOM	2800	C	LYS	A	363	49.969	12.635	35.476	1.00	59.79	C
ATOM	2801	O	LYS	A	363	49.812	12.679	34.230	1.00	59.78	O
ATOM	2802	N	VAL	A	364	51.047	13.133	36.088	1.00	59.02	N
ATOM	2803	CA	VAL	A	364	52.181	13.708	35.371	1.00	58.14	C
ATOM	2804	CB	VAL	A	364	53.022	14.587	36.278	1.00	58.03	C
ATOM	2805	CG1	VAL	A	364	53.647	15.678	35.453	1.00	58.99	C
ATOM	2806	CG2	VAL	A	364	52.194	15.174	37.428	1.00	58.01	C
ATOM	2807	C	VAL	A	364	53.097	12.639	34.808	1.00	57.69	C
ATOM	2808	O	VAL	A	364	54.049	12.231	35.459	1.00	57.73	O
ATOM	2809	N	THR	A	365	52.801	12.199	33.593	1.00	57.33	N
ATOM	2810	CA	THR	A	365	53.507	11.104	32.933	1.00	57.15	C
ATOM	2811	CB	THR	A	365	52.813	9.797	33.231	1.00	57.12	C
ATOM	2812	OG1	THR	A	365	52.848	9.551	34.645	1.00	57.01	O
ATOM	2813	CG2	THR	A	365	53.557	8.624	32.569	1.00	56.35	C
ATOM	2814	C	THR	A	365	53.380	11.349	31.455	1.00	57.41	C
ATOM	2815	O	THR	A	365	52.320	11.800	31.018	1.00	58.15	O
ATOM	2816	N	MET	A	366	54.427	11.040	30.682	1.00	57.38	N
ATOM	2817	CA	MET	A	366	54.488	11.347	29.230	1.00	56.93	C
ATOM	2818	CB	MET	A	366	55.851	10.938	28.635	1.00	57.08	C
ATOM	2819	CG	MET	A	366	55.891	10.103	27.344	1.00	55.95	C
ATOM	2820	SD	MET	A	366	56.806	11.131	26.205	1.00	54.10	S
ATOM	2821	CE	MET	A	366	57.071	9.996	24.722	1.00	55.24	C
ATOM	2822	C	MET	A	366	53.313	10.677	28.542	1.00	56.83	C
ATOM	2823	O	MET	A	366	52.874	11.100	27.463	1.00	56.70	O
ATOM	2824	N	ASP	A	367	52.798	9.642	29.210	1.00	56.23	N
ATOM	2825	CA	ASP	A	367	51.415	9.246	29.015	1.00	55.59	C
ATOM	2826	CB	ASP	A	367	51.151	7.871	29.579	1.00	55.62	C
ATOM	2827	CG	ASP	A	367	51.307	6.835	28.521	1.00	56.76	C
ATOM	2828	OD1	ASP	A	367	51.564	5.625	28.819	1.00	57.98	O
ATOM	2829	OD2	ASP	A	367	51.201	7.202	27.323	1.00	57.12	O
ATOM	2830	C	ASP	A	367	50.408	10.329	29.453	1.00	54.85	C
ATOM	2831	O	ASP	A	367	50.260	11.320	28.739	1.00	54.58	O
ATOM	2832	N	ASP	A	368	49.740	10.214	30.595	1.00	53.69	N
ATOM	2833	CA	ASP	A	368	48.678	11.192	30.852	1.00	52.80	C
ATOM	2834	CB	ASP	A	368	48.272	11.263	32.346	1.00	52.77	C
ATOM	2835	CG	ASP	A	368	47.202	10.169	32.753	1.00	54.13	C
ATOM	2836	OD1	ASP	A	368	46.702	9.412	31.865	1.00	53.72	O
ATOM	2837	OD2	ASP	A	368	46.802	9.988	33.948	1.00	54.20	O
ATOM	2838	C	ASP	A	368	48.949	12.577	30.176	1.00	51.86	C
ATOM	2839	O	ASP	A	368	48.125	13.487	30.264	1.00	52.51	O
ATOM	2840	N	PHE	A	369	50.078	12.705	29.470	1.00	50.15	N
ATOM	2841	CA	PHE	A	369	50.374	13.857	28.601	1.00	49.24	C
ATOM	2842	CB	PHE	A	369	51.901	14.088	28.508	1.00	49.50	C
ATOM	2843	CG	PHE	A	369	52.334	15.035	27.393	1.00	50.20	C
ATOM	2844	CD1	PHE	A	369	52.839	14.536	26.180	1.00	52.35	C
ATOM	2845	CE1	PHE	A	369	53.247	15.413	25.137	1.00	52.29	C
ATOM	2846	CZ	PHE	A	369	53.160	16.796	25.328	1.00	51.28	C
ATOM	2847	CE2	PHE	A	369	52.661	17.293	26.536	1.00	49.84	C
ATOM	2848	CD2	PHE	A	369	52.258	16.413	27.558	1.00	49.23	C
ATOM	2849	C	PHE	A	369	49.782	13.603	27.216	1.00	48.23	C
ATOM	2850	O	PHE	A	369	48.706	14.096	26.869	1.00	48.04	O
ATOM	2851	N	LEU	A	370	50.535	12.842	26.429	1.00	46.91	N
ATOM	2852	CA	LEU	A	370	50.067	12.159	25.236	1.00	45.61	C
ATOM	2853	CB	LEU	A	370	50.931	10.929	25.056	1.00	45.48	C

252/396

Figure 3A-52

ATOM	2854	CG	LEU	A	370	52.178	11.096	24.237	1.00	45.15	C
ATOM	2855	CD1	LEU	A	370	52.678	9.680	23.826	1.00	44.87	C
ATOM	2856	CD2	LEU	A	370	51.919	12.025	23.048	1.00	44.23	C
ATOM	2857	C	LEU	A	370	48.594	11.667	25.205	1.00	44.97	C
ATOM	2858	O	LEU	A	370	48.055	11.447	24.112	1.00	44.60	O
ATOM	2859	N	THR	A	371	47.970	11.432	26.371	1.00	43.75	N
ATOM	2860	CA	THR	A	371	46.559	11.025	26.384	1.00	42.24	C
ATOM	2861	CB	THR	A	371	46.195	10.006	27.512	1.00	42.10	C
ATOM	2862	OG1	THR	A	371	46.546	8.686	27.072	1.00	41.39	O
ATOM	2863	CG2	THR	A	371	44.676	9.880	27.679	1.00	40.74	C
ATOM	2864	C	THR	A	371	45.651	12.243	26.358	1.00	41.30	C
ATOM	2865	O	THR	A	371	44.851	12.425	25.429	1.00	41.29	O
ATOM	2866	N	ALA	A	372	45.790	13.103	27.341	1.00	39.83	N
ATOM	2867	CA	ALA	A	372	45.008	14.306	27.288	1.00	38.66	C
ATOM	2868	CB	ALA	A	372	45.297	15.148	28.459	1.00	39.14	C
ATOM	2869	C	ALA	A	372	45.326	15.032	25.993	1.00	37.65	C
ATOM	2870	O	ALA	A	372	44.898	16.133	25.778	1.00	36.93	O
ATOM	2871	N	HIS	A	373	46.081	14.400	25.119	1.00	37.44	N
ATOM	2872	CA	HIS	A	373	46.314	14.997	23.808	1.00	37.97	C
ATOM	2873	CB	HIS	A	373	47.686	14.640	23.247	1.00	38.17	C
ATOM	2874	CG	HIS	A	373	48.526	15.833	22.940	1.00	38.59	C
ATOM	2875	ND1	HIS	A	373	48.805	16.807	23.884	1.00	38.30	N
ATOM	2876	CE1	HIS	A	373	49.575	17.728	23.338	1.00	39.08	C
ATOM	2877	NE2	HIS	A	373	49.818	17.377	22.084	1.00	39.70	N
ATOM	2878	CD2	HIS	A	373	49.165	16.200	21.807	1.00	37.80	C
ATOM	2879	C	HIS	A	373	45.318	14.497	22.824	1.00	37.57	C
ATOM	2880	O	HIS	A	373	45.027	15.158	21.825	1.00	38.18	O
ATOM	2881	N	HIS	A	374	44.866	13.278	23.072	1.00	36.56	N
ATOM	2882	CA	HIS	A	374	43.918	12.649	22.208	1.00	35.05	C
ATOM	2883	CB	HIS	A	374	44.293	11.202	22.009	1.00	34.83	C
ATOM	2884	CG	HIS	A	374	43.169	10.252	22.210	1.00	34.87	C
ATOM	2885	ND1	HIS	A	374	43.208	8.959	21.742	1.00	35.52	N
ATOM	2886	CE1	HIS	A	374	42.079	8.352	22.056	1.00	36.37	C
ATOM	2887	NE2	HIS	A	374	41.308	9.210	22.705	1.00	35.85	N
ATOM	2888	CD2	HIS	A	374	41.970	10.402	22.817	1.00	35.07	C
ATOM	2889	C	HIS	A	374	42.581	12.841	22.896	1.00	34.34	C
ATOM	2890	O	HIS	A	374	41.597	13.162	22.225	1.00	34.49	O
ATOM	2891	N	GLU	A	375	42.539	12.707	24.221	1.00	32.89	N
ATOM	2892	CA	GLU	A	375	41.358	13.147	24.940	1.00	32.18	C
ATOM	2893	CB	GLU	A	375	41.600	13.180	26.431	1.00	31.64	C
ATOM	2894	CG	GLU	A	375	41.407	11.825	27.035	1.00	31.72	C
ATOM	2895	CD	GLU	A	375	40.383	11.038	26.247	1.00	34.26	C
ATOM	2896	OE1	GLU	A	375	39.189	11.326	26.398	1.00	36.46	O
ATOM	2897	OE2	GLU	A	375	40.736	10.137	25.456	1.00	35.91	O
ATOM	2898	C	GLU	A	375	40.924	14.506	24.392	1.00	32.47	C
ATOM	2899	O	GLU	A	375	39.763	14.706	24.013	1.00	32.81	O
ATOM	2900	N	MET	A	376	41.872	15.426	24.265	1.00	32.48	N
ATOM	2901	CA	MET	A	376	41.592	16.687	23.588	1.00	32.49	C
ATOM	2902	CB	MET	A	376	42.681	17.698	23.892	1.00	32.49	C
ATOM	2903	CG	MET	A	376	42.154	19.069	24.089	1.00	32.96	C
ATOM	2904	SD	MET	A	376	43.406	20.232	24.668	1.00	37.36	S
ATOM	2905	CE	MET	A	376	43.180	20.025	26.514	1.00	33.60	C
ATOM	2906	C	MET	A	376	41.404	16.551	22.060	1.00	32.52	C
ATOM	2907	O	MET	A	376	41.329	17.552	21.336	1.00	32.57	O
ATOM	2908	N	GLY	A	377	41.355	15.326	21.554	1.00	32.18	N
ATOM	2909	CA	GLY	A	377	41.093	15.155	20.145	1.00	32.37	C

253/396

Figure 3A-53

ATOM	2910	C	GLY	A	377	39.604	15.342	20.072	1.00	32.51	C
ATOM	2911	O	GLY	A	377	39.039	16.220	19.376	1.00	31.73	O
ATOM	2912	N	HIS	A	378	38.985	14.511	20.892	1.00	32.48	N
ATOM	2913	CA	HIS	A	378	37.566	14.443	21.003	1.00	32.60	C
ATOM	2914	CB	HIS	A	378	37.251	13.552	22.129	1.00	32.14	C
ATOM	2915	CG	HIS	A	378	37.293	12.153	21.703	1.00	34.34	C
ATOM	2916	ND1	HIS	A	378	37.379	11.824	20.372	1.00	35.19	N
ATOM	2917	CE1	HIS	A	378	37.383	10.511	20.246	1.00	38.12	C
ATOM	2918	NE2	HIS	A	378	37.319	9.980	21.455	1.00	41.28	N
ATOM	2919	CD2	HIS	A	378	37.261	10.991	22.388	1.00	39.05	C
ATOM	2920	C	HIS	A	378	36.855	15.752	21.128	1.00	32.65	C
ATOM	2921	O	HIS	A	378	35.844	15.988	20.449	1.00	33.35	O
ATOM	2922	N	ILE	A	379	37.361	16.628	21.965	1.00	31.59	N
ATOM	2923	CA	ILE	A	379	36.642	17.840	22.069	1.00	30.99	C
ATOM	2924	CB	ILE	A	379	37.202	18.633	23.180	1.00	30.66	C
ATOM	2925	CG1	ILE	A	379	37.008	17.873	24.504	1.00	31.39	C
ATOM	2926	CD1	ILE	A	379	35.868	16.796	24.547	1.00	31.86	C
ATOM	2927	CG2	ILE	A	379	36.566	20.003	23.219	1.00	30.81	C
ATOM	2928	C	ILE	A	379	36.816	18.483	20.715	1.00	31.23	C
ATOM	2929	O	ILE	A	379	35.863	18.842	20.059	1.00	31.47	O
ATOM	2930	N	GLN	A	380	38.038	18.540	20.235	1.00	31.61	N
ATOM	2931	CA	GLN	A	380	38.294	19.373	19.081	1.00	31.70	C
ATOM	2932	CB	GLN	A	380	39.742	19.224	18.618	1.00	32.01	C
ATOM	2933	CG	GLN	A	380	40.249	20.438	17.900	1.00	30.55	C
ATOM	2934	CD	GLN	A	380	40.190	21.642	18.770	1.00	30.08	C
ATOM	2935	OE1	GLN	A	380	40.179	22.741	18.258	1.00	32.75	O
ATOM	2936	NE2	GLN	A	380	40.138	21.453	20.091	1.00	28.29	N
ATOM	2937	C	GLN	A	380	37.360	19.001	17.968	1.00	31.60	C
ATOM	2938	O	GLN	A	380	36.977	19.842	17.176	1.00	31.47	O
ATOM	2939	N	TYR	A	381	37.039	17.716	17.921	1.00	31.55	N
ATOM	2940	CA	TYR	A	381	36.112	17.152	16.962	1.00	31.58	C
ATOM	2941	CB	TYR	A	381	36.312	15.623	16.925	1.00	30.69	C
ATOM	2942	CG	TYR	A	381	35.932	14.903	15.655	1.00	26.97	C
ATOM	2943	CD1	TYR	A	381	35.571	13.577	15.684	1.00	26.48	C
ATOM	2944	CE1	TYR	A	381	35.183	12.882	14.504	1.00	27.90	C
ATOM	2945	CZ	TYR	A	381	35.169	13.542	13.277	1.00	26.61	C
ATOM	2946	OH	TYR	A	381	34.811	12.879	12.098	1.00	26.00	O
ATOM	2947	CE2	TYR	A	381	35.556	14.862	13.244	1.00	25.82	C
ATOM	2948	CD2	TYR	A	381	35.953	15.529	14.432	1.00	24.94	C
ATOM	2949	C	TYR	A	381	34.718	17.537	17.458	1.00	32.81	C
ATOM	2950	O	TYR	A	381	34.032	18.386	16.867	1.00	32.22	O
ATOM	2951	N	ASP	A	382	34.317	16.947	18.573	1.00	34.62	N
ATOM	2952	CA	ASP	A	382	33.074	17.326	19.220	1.00	37.05	C
ATOM	2953	CB	ASP	A	382	33.128	16.970	20.715	1.00	37.42	C
ATOM	2954	CG	ASP	A	382	32.628	15.531	20.992	1.00	40.99	C
ATOM	2955	OD1	ASP	A	382	31.405	15.344	20.771	1.00	45.70	O
ATOM	2956	OD2	ASP	A	382	33.327	14.534	21.404	1.00	40.58	O
ATOM	2957	C	ASP	A	382	32.672	18.806	18.950	1.00	37.96	C
ATOM	2958	O	ASP	A	382	31.498	19.082	18.677	1.00	38.97	O
ATOM	2959	N	MET	A	383	33.650	19.723	18.982	1.00	38.31	N
ATOM	2960	CA	MET	A	383	33.460	21.163	18.823	1.00	38.20	C
ATOM	2961	CB	MET	A	383	34.791	21.874	19.018	1.00	38.46	C
ATOM	2962	CG	MET	A	383	35.552	21.603	20.284	1.00	40.56	C
ATOM	2963	SD	MET	A	383	35.785	23.083	21.348	1.00	45.76	S
ATOM	2964	CE	MET	A	383	34.798	24.418	20.393	1.00	43.45	C
ATOM	2965	C	MET	A	383	33.084	21.484	17.416	1.00	38.25	C

254/396

Figure 3A-54

ATOM	2966	O	MET	A	383	32.178	22.276	17.135	1.00	37.89	O
ATOM	2967	N	ALA	A	384	33.888	20.914	16.528	1.00	39.00	N
ATOM	2968	CA	ALA	A	384	33.848	21.190	15.108	1.00	39.39	C
ATOM	2969	CB	ALA	A	384	34.850	20.317	14.366	1.00	38.91	C
ATOM	2970	C	ALA	A	384	32.479	20.749	14.749	1.00	39.65	C
ATOM	2971	O	ALA	A	384	31.638	21.524	14.258	1.00	40.27	O
ATOM	2972	N	TYR	A	385	32.230	19.491	15.037	1.00	39.41	N
ATOM	2973	CA	TYR	A	385	31.051	18.911	14.457	1.00	39.24	C
ATOM	2974	CB	TYR	A	385	31.222	17.368	14.239	1.00	38.99	C
ATOM	2975	CG	TYR	A	385	31.185	16.468	15.460	1.00	36.27	C
ATOM	2976	CD1	TYR	A	385	31.445	15.115	15.339	1.00	32.32	C
ATOM	2977	CE1	TYR	A	385	31.390	14.311	16.417	1.00	32.37	C
ATOM	2978	CZ	TYR	A	385	31.082	14.858	17.655	1.00	35.23	C
ATOM	2979	OH	TYR	A	385	30.994	14.071	18.775	1.00	39.67	O
ATOM	2980	CE2	TYR	A	385	30.816	16.190	17.808	1.00	34.42	C
ATOM	2981	CD2	TYR	A	385	30.868	16.979	16.721	1.00	35.61	C
ATOM	2982	C	TYR	A	385	29.721	19.429	15.091	1.00	39.29	C
ATOM	2983	O	TYR	A	385	28.653	19.110	14.607	1.00	40.07	O
ATOM	2984	N	ALA	A	386	29.772	20.282	16.113	1.00	39.03	N
ATOM	2985	CA	ALA	A	386	28.517	20.836	16.658	1.00	38.78	C
ATOM	2986	CB	ALA	A	386	28.693	21.294	18.082	1.00	38.85	C
ATOM	2987	C	ALA	A	386	27.855	21.935	15.794	1.00	38.62	C
ATOM	2988	O	ALA	A	386	27.180	22.834	16.287	1.00	38.72	O
ATOM	2989	N	ALA	A	387	28.035	21.836	14.495	1.00	38.36	N
ATOM	2990	CA	ALA	A	387	27.336	22.692	13.579	1.00	38.27	C
ATOM	2991	CB	ALA	A	387	28.349	23.537	12.805	1.00	38.10	C
ATOM	2992	C	ALA	A	387	26.525	21.774	12.653	1.00	38.23	C
ATOM	2993	O	ALA	A	387	25.964	22.193	11.635	1.00	38.97	O
ATOM	2994	N	GLN	A	388	26.474	20.499	13.000	1.00	37.47	N
ATOM	2995	CA	GLN	A	388	25.710	19.563	12.212	1.00	36.98	C
ATOM	2996	CB	GLN	A	388	26.216	18.145	12.432	1.00	36.52	C
ATOM	2997	CG	GLN	A	388	26.964	17.582	11.260	1.00	34.81	C
ATOM	2998	CD	GLN	A	388	27.211	18.598	10.142	1.00	34.08	C
ATOM	2999	OE1	GLN	A	388	27.241	18.211	8.992	1.00	35.22	O
ATOM	3000	NE2	GLN	A	388	27.411	19.877	10.476	1.00	31.95	N
ATOM	3001	C	GLN	A	388	24.329	19.679	12.740	1.00	37.54	C
ATOM	3002	O	GLN	A	388	24.134	20.347	13.735	1.00	38.21	O
ATOM	3003	N	PRO	A	389	23.357	19.071	12.079	1.00	37.69	N
ATOM	3004	CA	PRO	A	389	22.064	18.799	12.704	1.00	37.73	C
ATOM	3005	CB	PRO	A	389	21.304	18.127	11.568	1.00	37.90	C
ATOM	3006	CG	PRO	A	389	22.405	17.470	10.769	1.00	37.66	C
ATOM	3007	CD	PRO	A	389	23.396	18.615	10.679	1.00	37.89	C
ATOM	3008	C	PRO	A	389	22.257	17.787	13.831	1.00	38.11	C
ATOM	3009	O	PRO	A	389	22.229	16.600	13.500	1.00	38.09	O
ATOM	3010	N	PHE	A	390	22.422	18.221	15.095	1.00	38.68	N
ATOM	3011	CA	PHE	A	390	22.780	17.331	16.243	1.00	39.21	C
ATOM	3012	CB	PHE	A	390	22.069	17.713	17.565	1.00	38.58	C
ATOM	3013	CG	PHE	A	390	21.483	16.518	18.324	1.00	38.88	C
ATOM	3014	CD1	PHE	A	390	21.648	16.397	19.708	1.00	40.48	C
ATOM	3015	CE1	PHE	A	390	21.059	15.258	20.429	1.00	40.23	C
ATOM	3016	CZ	PHE	A	390	20.327	14.262	19.728	1.00	37.43	C
ATOM	3017	CE2	PHE	A	390	20.162	14.400	18.344	1.00	36.88	C
ATOM	3018	CD2	PHE	A	390	20.721	15.522	17.662	1.00	37.20	C
ATOM	3019	C	PHE	A	390	22.620	15.830	16.000	1.00	39.79	C
ATOM	3020	O	PHE	A	390	23.520	15.046	16.348	1.00	39.40	O
ATOM	3021	N	LEU	A	391	21.463	15.465	15.420	1.00	40.46	N

255/396

Figure 3A-55

ATOM	3022	CA	LEU	A	391	21.044	14.089	15.161	1.00	41.49	C
ATOM	3023	CB	LEU	A	391	19.686	14.119	14.441	1.00	42.11	C
ATOM	3024	CG	LEU	A	391	18.632	12.968	14.569	1.00	44.61	C
ATOM	3025	CD1	LEU	A	391	18.090	12.616	13.143	1.00	46.03	C
ATOM	3026	CD2	LEU	A	391	19.016	11.649	15.402	1.00	42.29	C
ATOM	3027	C	LEU	A	391	22.076	13.267	14.369	1.00	41.31	C
ATOM	3028	O	LEU	A	391	21.762	12.230	13.775	1.00	41.04	O
ATOM	3029	N	LEU	A	392	23.324	13.716	14.413	1.00	41.14	N
ATOM	3030	CA	LEU	A	392	24.265	13.334	13.409	1.00	41.11	C
ATOM	3031	CB	LEU	A	392	23.542	13.373	12.106	1.00	40.81	C
ATOM	3032	CG	LEU	A	392	23.902	12.372	11.072	1.00	41.19	C
ATOM	3033	CD1	LEU	A	392	23.068	11.103	11.260	1.00	41.64	C
ATOM	3034	CD2	LEU	A	392	23.545	13.111	9.798	1.00	42.76	C
ATOM	3035	C	LEU	A	392	25.399	14.338	13.359	1.00	41.88	C
ATOM	3036	O	LEU	A	392	25.663	14.944	12.305	1.00	42.80	O
ATOM	3037	N	ARG	A	393	26.028	14.545	14.521	1.00	42.10	N
ATOM	3038	CA	ARG	A	393	27.416	15.028	14.662	1.00	41.29	C
ATOM	3039	CB	ARG	A	393	27.424	16.259	15.528	1.00	41.13	C
ATOM	3040	CG	ARG	A	393	26.035	16.599	15.955	1.00	41.08	C
ATOM	3041	CD	ARG	A	393	25.939	17.763	16.838	1.00	42.25	C
ATOM	3042	NE	ARG	A	393	25.737	18.988	16.080	1.00	41.92	N
ATOM	3043	CZ	ARG	A	393	25.029	20.017	16.511	1.00	42.52	C
ATOM	3044	NH1	ARG	A	393	24.414	19.971	17.690	1.00	41.84	N
ATOM	3045	NH2	ARG	A	393	24.937	21.101	15.753	1.00	44.61	N
ATOM	3046	C	ARG	A	393	28.101	13.867	15.373	1.00	41.12	C
ATOM	3047	O	ARG	A	393	27.811	13.546	16.534	1.00	40.68	O
ATOM	3048	N	ASN	A	394	28.951	13.160	14.665	1.00	41.02	N
ATOM	3049	CA	ASN	A	394	29.257	11.872	15.191	1.00	41.41	C
ATOM	3050	CB	ASN	A	394	28.006	11.016	15.183	1.00	41.91	C
ATOM	3051	CG	ASN	A	394	27.888	10.220	16.417	1.00	44.95	C
ATOM	3052	OD1	ASN	A	394	27.467	10.747	17.448	1.00	48.56	O
ATOM	3053	ND2	ASN	A	394	28.318	8.945	16.365	1.00	47.44	N
ATOM	3054	C	ASN	A	394	30.326	11.157	14.457	1.00	41.20	C
ATOM	3055	O	ASN	A	394	30.268	9.914	14.321	1.00	41.25	O
ATOM	3056	N	GLY	A	395	31.312	11.929	14.006	1.00	40.81	N
ATOM	3057	CA	GLY	A	395	32.479	11.376	13.348	1.00	40.43	C
ATOM	3058	C	GLY	A	395	32.112	10.536	12.131	1.00	40.36	C
ATOM	3059	O	GLY	A	395	31.064	9.880	12.085	1.00	40.41	O
ATOM	3060	N	ALA	A	396	32.981	10.538	11.132	1.00	39.87	N
ATOM	3061	CA	ALA	A	396	32.678	9.837	9.906	1.00	39.27	C
ATOM	3062	CB	ALA	A	396	33.788	10.016	8.986	1.00	39.78	C
ATOM	3063	C	ALA	A	396	32.460	8.369	10.154	1.00	39.06	C
ATOM	3064	O	ALA	A	396	31.960	7.669	9.297	1.00	39.32	O
ATOM	3065	N	ASN	A	397	32.834	7.940	11.355	1.00	39.02	N
ATOM	3066	CA	ASN	A	397	32.935	6.555	11.787	1.00	38.77	C
ATOM	3067	CB	ASN	A	397	33.605	5.724	10.725	1.00	39.10	C
ATOM	3068	CG	ASN	A	397	34.813	5.025	11.252	1.00	40.87	C
ATOM	3069	OD1	ASN	A	397	34.691	3.926	11.768	1.00	44.08	O
ATOM	3070	ND2	ASN	A	397	35.983	5.678	11.196	1.00	41.45	N
ATOM	3071	C	ASN	A	397	33.867	6.569	12.989	1.00	38.45	C
ATOM	3072	O	ASN	A	397	34.842	7.344	13.003	1.00	37.54	O
ATOM	3073	N	GLU	A	398	33.611	5.696	13.971	1.00	38.63	N
ATOM	3074	CA	GLU	A	398	34.444	5.651	15.197	1.00	38.86	C
ATOM	3075	CB	GLU	A	398	34.248	4.355	16.054	1.00	38.43	C
ATOM	3076	CG	GLU	A	398	34.111	3.022	15.306	1.00	40.04	C
ATOM	3077	CD	GLU	A	398	33.447	1.880	16.132	1.00	42.94	C

256/396

Figure 3A-56

ATOM	3078	OE1	GLU	A	398	32.685	2.229	17.074	1.00	42.63	O
ATOM	3079	OE2	GLU	A	398	33.672	0.632	15.846	1.00	40.94	O
ATOM	3080	C	GLU	A	398	35.949	6.021	14.907	1.00	38.56	C
ATOM	3081	O	GLU	A	398	36.382	7.161	15.222	1.00	38.13	O
ATOM	3082	N	GLY	A	399	36.708	5.106	14.273	1.00	37.62	N
ATOM	3083	CA	GLY	A	399	38.094	5.362	13.871	1.00	35.83	C
ATOM	3084	C	GLY	A	399	38.419	6.839	13.679	1.00	34.56	C
ATOM	3085	O	GLY	A	399	39.322	7.389	14.306	1.00	34.00	O
ATOM	3086	N	PHE	A	400	37.654	7.491	12.819	1.00	33.41	N
ATOM	3087	CA	PHE	A	400	37.746	8.925	12.725	1.00	32.20	C
ATOM	3088	CB	PHE	A	400	36.639	9.494	11.831	1.00	31.65	C
ATOM	3089	CG	PHE	A	400	36.984	9.506	10.362	1.00	29.15	C
ATOM	3090	CD1	PHE	A	400	37.107	8.303	9.639	1.00	26.20	C
ATOM	3091	CE1	PHE	A	400	37.407	8.301	8.274	1.00	23.71	C
ATOM	3092	CZ	PHE	A	400	37.597	9.501	7.608	1.00	22.62	C
ATOM	3093	CE2	PHE	A	400	37.491	10.709	8.316	1.00	24.71	C
ATOM	3094	CD2	PHE	A	400	37.176	10.709	9.694	1.00	25.96	C
ATOM	3095	C	PHE	A	400	37.656	9.542	14.112	1.00	32.09	C
ATOM	3096	O	PHE	A	400	38.390	10.470	14.433	1.00	31.83	O
ATOM	3097	N	HIS	A	401	36.760	9.068	14.960	1.00	32.05	N
ATOM	3098	CA	HIS	A	401	36.660	9.812	16.204	1.00	32.42	C
ATOM	3099	CB	HIS	A	401	35.362	9.633	16.996	1.00	32.72	C
ATOM	3100	CG	HIS	A	401	34.818	10.929	17.520	1.00	31.77	C
ATOM	3101	ND1	HIS	A	401	35.631	11.970	17.908	1.00	31.67	N
ATOM	3102	CE1	HIS	A	401	34.898	12.992	18.305	1.00	29.99	C
ATOM	3103	NE2	HIS	A	401	33.632	12.653	18.179	1.00	32.38	N
ATOM	3104	CD2	HIS	A	401	33.552	11.369	17.684	1.00	31.64	C
ATOM	3105	C	HIS	A	401	37.852	9.527	17.033	1.00	32.59	C
ATOM	3106	O	HIS	A	401	38.512	10.461	17.477	1.00	33.29	O
ATOM	3107	N	GLU	A	402	38.171	8.239	17.161	1.00	32.56	N
ATOM	3108	CA	GLU	A	402	39.323	7.753	17.951	1.00	32.01	C
ATOM	3109	CB	GLU	A	402	39.218	6.244	18.124	1.00	31.27	C
ATOM	3110	CG	GLU	A	402	38.125	5.846	19.088	1.00	29.67	C
ATOM	3111	CD	GLU	A	402	38.422	6.355	20.461	1.00	25.46	C
ATOM	3112	OE1	GLU	A	402	39.171	7.354	20.521	1.00	22.53	O
ATOM	3113	OE2	GLU	A	402	37.939	5.753	21.448	1.00	22.64	O
ATOM	3114	C	GLU	A	402	40.722	8.053	17.422	1.00	32.35	C
ATOM	3115	O	GLU	A	402	41.671	7.551	17.973	1.00	32.45	O
ATOM	3116	N	ALA	A	403	40.850	8.877	16.390	1.00	32.67	N
ATOM	3117	CA	ALA	A	403	42.076	8.973	15.638	1.00	33.28	C
ATOM	3118	CB	ALA	A	403	41.877	8.332	14.293	1.00	33.19	C
ATOM	3119	C	ALA	A	403	42.560	10.398	15.455	1.00	33.96	C
ATOM	3120	O	ALA	A	403	43.607	10.649	14.867	1.00	34.15	O
ATOM	3121	N	VAL	A	404	41.802	11.352	15.932	1.00	34.90	N
ATOM	3122	CA	VAL	A	404	42.082	12.694	15.479	1.00	36.12	C
ATOM	3123	CB	VAL	A	404	40.759	13.541	15.372	1.00	36.01	C
ATOM	3124	CG1	VAL	A	404	39.962	13.580	16.725	1.00	34.28	C
ATOM	3125	CG2	VAL	A	404	41.024	14.928	14.772	1.00	35.02	C
ATOM	3126	C	VAL	A	404	43.135	13.184	16.458	1.00	37.69	C
ATOM	3127	O	VAL	A	404	43.752	14.253	16.301	1.00	37.64	O
ATOM	3128	N	GLY	A	405	43.346	12.343	17.473	1.00	39.65	N
ATOM	3129	CA	GLY	A	405	44.261	12.636	18.579	1.00	41.63	C
ATOM	3130	C	GLY	A	405	45.569	11.935	18.295	1.00	42.43	C
ATOM	3131	O	GLY	A	405	46.542	12.577	17.887	1.00	42.74	O
ATOM	3132	N	ALA	A	406	45.594	10.617	18.467	1.00	42.85	N
ATOM	3133	CA	ALA	A	406	46.697	9.872	17.921	1.00	43.44	C

257/396

Figure 3A-57

ATOM	3134	CB	ALA	A	406	46.224	8.509	17.410	1.00	43.19	C
ATOM	3135	C	ALA	A	406	47.409	10.743	16.831	1.00	43.98	C
ATOM	3136	O	ALA	A	406	48.613	10.935	16.943	1.00	44.06	O
ATOM	3137	N	ILE	A	407	46.685	11.337	15.860	1.00	44.80	N
ATOM	3138	CA	ILE	A	407	47.310	12.217	14.829	1.00	46.19	C
ATOM	3139	CB	ILE	A	407	46.284	12.870	13.859	1.00	46.39	C
ATOM	3140	CG1	ILE	A	407	45.974	11.928	12.695	1.00	47.88	C
ATOM	3141	CD1	ILE	A	407	44.487	11.508	12.570	1.00	49.85	C
ATOM	3142	CG2	ILE	A	407	46.809	14.228	13.288	1.00	45.25	C
ATOM	3143	C	ILE	A	407	48.214	13.313	15.374	1.00	47.15	C
ATOM	3144	O	ILE	A	407	49.306	13.543	14.831	1.00	47.62	O
ATOM	3145	N	MET	A	408	47.743	14.013	16.407	1.00	47.95	N
ATOM	3146	CA	MET	A	408	48.551	15.006	17.107	1.00	48.79	C
ATOM	3147	CB	MET	A	408	47.692	15.831	18.038	1.00	49.47	C
ATOM	3148	CG	MET	A	408	46.480	16.397	17.362	1.00	53.02	C
ATOM	3149	SD	MET	A	408	46.868	18.027	16.682	1.00	61.10	S
ATOM	3150	CE	MET	A	408	47.519	17.535	15.027	1.00	61.30	C
ATOM	3151	C	MET	A	408	49.679	14.311	17.853	1.00	48.55	C
ATOM	3152	O	MET	A	408	50.791	14.313	17.360	1.00	48.90	O
ATOM	3153	N	SER	A	409	49.402	13.696	19.006	1.00	48.21	N
ATOM	3154	CA	SER	A	409	50.366	12.812	19.681	1.00	48.20	C
ATOM	3155	CB	SER	A	409	49.682	11.523	20.119	1.00	48.32	C
ATOM	3156	OG	SER	A	409	48.491	11.821	20.812	1.00	49.39	O
ATOM	3157	C	SER	A	409	51.549	12.425	18.807	1.00	48.02	C
ATOM	3158	O	SER	A	409	52.695	12.617	19.203	1.00	47.78	O
ATOM	3159	N	LEU	A	410	51.236	11.883	17.623	1.00	47.77	N
ATOM	3160	CA	LEU	A	410	52.201	11.468	16.610	1.00	47.56	C
ATOM	3161	CB	LEU	A	410	51.496	11.165	15.286	1.00	47.21	C
ATOM	3162	CG	LEU	A	410	51.864	9.932	14.430	1.00	46.24	C
ATOM	3163	CD1	LEU	A	410	53.264	9.413	14.671	1.00	44.87	C
ATOM	3164	CD2	LEU	A	410	50.853	8.817	14.647	1.00	44.44	C
ATOM	3165	C	LEU	A	410	53.280	12.509	16.357	1.00	48.06	C
ATOM	3166	O	LEU	A	410	54.468	12.173	16.215	1.00	48.69	O
ATOM	3167	N	SER	A	411	52.876	13.766	16.254	1.00	48.01	N
ATOM	3168	CA	SER	A	411	53.844	14.846	16.182	1.00	47.82	C
ATOM	3169	CB	SER	A	411	53.170	16.156	15.771	1.00	47.80	C
ATOM	3170	OG	SER	A	411	53.944	16.871	14.836	1.00	46.64	O
ATOM	3171	C	SER	A	411	54.413	14.959	17.574	1.00	47.92	C
ATOM	3172	O	SER	A	411	55.540	14.583	17.823	1.00	47.63	O
ATOM	3173	N	ALA	A	412	53.595	15.430	18.492	1.00	48.75	N
ATOM	3174	CA	ALA	A	412	54.024	15.667	19.854	1.00	50.15	C
ATOM	3175	CB	ALA	A	412	52.889	16.300	20.684	1.00	50.44	C
ATOM	3176	C	ALA	A	412	54.532	14.415	20.547	1.00	50.77	C
ATOM	3177	O	ALA	A	412	54.236	14.197	21.725	1.00	51.65	O
ATOM	3178	N	ALA	A	413	55.268	13.586	19.819	1.00	50.79	N
ATOM	3179	CA	ALA	A	413	56.095	12.575	20.438	1.00	51.00	C
ATOM	3180	CB	ALA	A	413	55.390	11.232	20.487	1.00	50.87	C
ATOM	3181	C	ALA	A	413	57.378	12.513	19.640	1.00	51.49	C
ATOM	3182	O	ALA	A	413	58.243	11.695	19.875	1.00	51.81	O
ATOM	3183	N	THR	A	414	57.526	13.399	18.686	1.00	52.24	N
ATOM	3184	CA	THR	A	414	58.828	13.528	18.094	1.00	53.36	C
ATOM	3185	CB	THR	A	414	58.749	14.299	16.770	1.00	53.37	C
ATOM	3186	OG1	THR	A	414	58.182	15.600	16.970	1.00	52.39	O
ATOM	3187	CG2	THR	A	414	57.740	13.640	15.886	1.00	54.50	C
ATOM	3188	C	THR	A	414	59.738	14.220	19.115	1.00	54.32	C
ATOM	3189	O	THR	A	414	59.324	15.191	19.765	1.00	54.36	O

258/396

Figure 3A-58

ATOM	3190	N	PRO	A	415	60.946	13.695	19.307	1.00	55.01	N
ATOM	3191	CA	PRO	A	415	61.973	14.431	20.013	1.00	55.59	C
ATOM	3192	CB	PRO	A	415	63.249	13.736	19.558	1.00	55.46	C
ATOM	3193	CG	PRO	A	415	62.857	12.330	19.406	1.00	55.14	C
ATOM	3194	CD	PRO	A	415	61.437	12.369	18.897	1.00	55.43	C
ATOM	3195	C	PRO	A	415	61.912	15.859	19.500	1.00	56.55	C
ATOM	3196	O	PRO	A	415	61.613	16.770	20.292	1.00	56.81	O
ATOM	3197	N	LYS	A	416	62.123	16.047	18.196	1.00	57.30	N
ATOM	3198	CA	LYS	A	416	62.071	17.383	17.588	1.00	58.31	C
ATOM	3199	CB	LYS	A	416	61.977	17.252	16.074	1.00	58.18	C
ATOM	3200	CG	LYS	A	416	61.311	18.423	15.402	1.00	59.63	C
ATOM	3201	CD	LYS	A	416	62.290	19.275	14.590	1.00	61.88	C
ATOM	3202	CE	LYS	A	416	61.531	20.245	13.667	1.00	62.22	C
ATOM	3203	NZ	LYS	A	416	60.771	19.548	12.566	1.00	61.24	N
ATOM	3204	C	LYS	A	416	60.951	18.315	18.139	1.00	58.71	C
ATOM	3205	O	LYS	A	416	61.080	19.551	18.167	1.00	58.01	O
ATOM	3206	N	HIS	A	417	59.856	17.718	18.581	1.00	59.81	N
ATOM	3207	CA	HIS	A	417	58.775	18.514	19.117	1.00	61.20	C
ATOM	3208	CB	HIS	A	417	57.405	17.864	18.876	1.00	61.65	C
ATOM	3209	CG	HIS	A	417	56.278	18.660	19.450	1.00	64.39	C
ATOM	3210	ND1	HIS	A	417	55.972	19.932	19.009	1.00	67.16	N
ATOM	3211	CE1	HIS	A	417	54.968	20.412	19.725	1.00	68.77	C
ATOM	3212	NE2	HIS	A	417	54.630	19.508	20.630	1.00	68.43	N
ATOM	3213	CD2	HIS	A	417	55.445	18.409	20.488	1.00	66.69	C
ATOM	3214	C	HIS	A	417	58.972	18.755	20.597	1.00	61.38	C
ATOM	3215	O	HIS	A	417	58.576	19.805	21.130	1.00	61.44	O
ATOM	3216	N	LEU	A	418	59.557	17.763	21.263	1.00	61.57	N
ATOM	3217	CA	LEU	A	418	59.681	17.796	22.705	1.00	61.81	C
ATOM	3218	CB	LEU	A	418	60.099	16.434	23.222	1.00	61.87	C
ATOM	3219	CG	LEU	A	418	59.040	15.346	23.450	1.00	61.54	C
ATOM	3220	CD1	LEU	A	418	57.733	15.913	24.008	1.00	62.07	C
ATOM	3221	CD2	LEU	A	418	58.800	14.543	22.188	1.00	60.32	C
ATOM	3222	C	LEU	A	418	60.693	18.841	23.074	1.00	62.34	C
ATOM	3223	O	LEU	A	418	60.666	19.385	24.177	1.00	62.15	O
ATOM	3224	N	LYS	A	419	61.579	19.119	22.122	1.00	63.33	N
ATOM	3225	CA	LYS	A	419	62.465	20.281	22.183	1.00	64.34	C
ATOM	3226	CB	LYS	A	419	63.527	20.212	21.064	1.00	64.67	C
ATOM	3227	CG	LYS	A	419	64.699	21.218	21.140	1.00	65.19	C
ATOM	3228	CD	LYS	A	419	65.444	21.305	19.787	1.00	66.35	C
ATOM	3229	CE	LYS	A	419	66.926	20.873	19.901	1.00	67.18	C
ATOM	3230	NZ	LYS	A	419	67.173	19.396	19.949	1.00	67.10	N
ATOM	3231	C	LYS	A	419	61.626	21.556	22.116	1.00	64.48	C
ATOM	3232	O	LYS	A	419	61.246	22.090	23.138	1.00	63.59	O
ATOM	3233	N	SER	A	420	61.323	22.021	20.916	1.00	65.79	N
ATOM	3234	CA	SER	A	420	60.369	23.113	20.738	1.00	67.57	C
ATOM	3235	CB	SER	A	420	59.453	22.857	19.508	1.00	68.26	C
ATOM	3236	OG	SER	A	420	58.246	22.121	19.806	1.00	69.21	O
ATOM	3237	C	SER	A	420	59.525	23.437	21.983	1.00	67.92	C
ATOM	3238	O	SER	A	420	59.272	24.604	22.262	1.00	67.64	O
ATOM	3239	N	ILE	A	421	59.076	22.412	22.712	1.00	68.92	N
ATOM	3240	CA	ILE	A	421	58.234	22.641	23.902	1.00	70.11	C
ATOM	3241	CB	ILE	A	421	57.144	21.451	24.118	1.00	69.77	C
ATOM	3242	CG1	ILE	A	421	55.817	21.992	24.650	1.00	69.26	C
ATOM	3243	CD1	ILE	A	421	54.868	22.532	23.560	1.00	68.55	C
ATOM	3244	CG2	ILE	A	421	57.627	20.313	24.991	1.00	69.92	C
ATOM	3245	C	ILE	A	421	59.085	23.132	25.145	1.00	70.96	C

259/396

Figure 3A-59

ATOM	3246	O	ILE	A	421	59.517	24.317	25.187	1.00	70.96	O
ATOM	3247	N	GLY	A	422	59.325	22.252	26.122	1.00	71.55	N
ATOM	3248	CA	GLY	A	422	60.368	22.451	27.119	1.00	71.85	C
ATOM	3249	C	GLY	A	422	61.053	21.111	27.216	1.00	72.08	C
ATOM	3250	O	GLY	A	422	61.824	20.715	26.342	1.00	71.53	O
ATOM	3251	N	LEU	A	423	60.745	20.415	28.298	1.00	72.72	N
ATOM	3252	CA	LEU	A	423	60.903	18.961	28.379	1.00	73.41	C
ATOM	3253	CB	LEU	A	423	59.824	18.274	27.516	1.00	73.41	C
ATOM	3254	CG	LEU	A	423	58.421	18.167	28.144	1.00	74.00	C
ATOM	3255	CD1	LEU	A	423	58.117	16.766	28.671	1.00	73.41	C
ATOM	3256	CD2	LEU	A	423	58.204	19.199	29.261	1.00	74.46	C
ATOM	3257	C	LEU	A	423	62.314	18.464	28.050	1.00	73.42	C
ATOM	3258	O	LEU	A	423	63.294	18.925	28.653	1.00	73.63	O
ATOM	3259	N	LEU	A	424	62.405	17.501	27.141	1.00	73.28	N
ATOM	3260	CA	LEU	A	424	63.654	17.216	26.483	1.00	73.77	C
ATOM	3261	CB	LEU	A	424	63.404	16.184	25.389	1.00	73.13	C
ATOM	3262	CG	LEU	A	424	64.448	16.061	24.294	1.00	72.25	C
ATOM	3263	CD1	LEU	A	424	64.973	14.647	24.254	1.00	72.10	C
ATOM	3264	CD2	LEU	A	424	63.844	16.485	22.978	1.00	70.94	C
ATOM	3265	C	LEU	A	424	64.226	18.553	25.922	1.00	74.71	C
ATOM	3266	O	LEU	A	424	63.731	19.052	24.909	1.00	75.00	O
ATOM	3267	N	SER	A	425	65.239	19.125	26.609	1.00	75.64	N
ATOM	3268	CA	SER	A	425	65.835	20.474	26.326	1.00	75.98	C
ATOM	3269	CB	SER	A	425	65.891	21.387	27.604	1.00	76.30	C
ATOM	3270	OG	SER	A	425	66.081	20.705	28.859	1.00	76.40	O
ATOM	3271	C	SER	A	425	67.205	20.449	25.572	1.00	75.96	C
ATOM	3272	O	SER	A	425	68.024	19.546	25.797	1.00	75.93	O
ATOM	3273	N	PRO	A	426	67.477	21.483	24.762	1.00	75.90	N
ATOM	3274	CA	PRO	A	426	68.341	21.395	23.564	1.00	75.91	C
ATOM	3275	CB	PRO	A	426	69.180	22.678	23.673	1.00	75.77	C
ATOM	3276	CG	PRO	A	426	68.374	23.600	24.647	1.00	75.71	C
ATOM	3277	CD	PRO	A	426	67.085	22.884	25.005	1.00	75.89	C
ATOM	3278	C	PRO	A	426	69.211	20.108	23.366	1.00	75.88	C
ATOM	3279	O	PRO	A	426	70.269	19.978	23.981	1.00	76.00	O
ATOM	3280	N	ASP	A	427	68.763	19.190	22.498	1.00	75.78	N
ATOM	3281	CA	ASP	A	427	69.305	17.810	22.440	1.00	75.48	C
ATOM	3282	CB	ASP	A	427	68.217	16.738	22.824	1.00	75.57	C
ATOM	3283	CG	ASP	A	427	67.772	15.804	21.643	1.00	75.33	C
ATOM	3284	OD1	ASP	A	427	67.864	16.210	20.456	1.00	76.03	O
ATOM	3285	OD2	ASP	A	427	67.292	14.648	21.822	1.00	72.22	O
ATOM	3286	C	ASP	A	427	70.121	17.440	21.183	1.00	75.25	C
ATOM	3287	O	ASP	A	427	69.923	17.997	20.092	1.00	74.87	O
ATOM	3288	N	ALA	A	428	71.006	16.463	21.391	1.00	75.05	N
ATOM	3289	CA	ALA	A	428	72.062	16.024	20.465	1.00	74.97	C
ATOM	3290	CB	ALA	A	428	72.826	14.834	21.091	1.00	75.12	C
ATOM	3291	C	ALA	A	428	71.693	15.720	18.989	1.00	74.75	C
ATOM	3292	O	ALA	A	428	71.283	14.586	18.676	1.00	74.52	O
ATOM	3293	N	ALA	A	429	71.941	16.720	18.110	1.00	74.42	N
ATOM	3294	CA	ALA	A	429	71.521	16.793	16.677	1.00	73.76	C
ATOM	3295	CB	ALA	A	429	72.721	16.795	15.742	1.00	73.38	C
ATOM	3296	C	ALA	A	429	70.463	15.750	16.249	1.00	73.37	C
ATOM	3297	O	ALA	A	429	69.298	16.095	15.934	1.00	73.91	O
ATOM	3298	N	ALA	A	430	70.883	14.487	16.238	1.00	71.64	N
ATOM	3299	CA	ALA	A	430	69.989	13.360	16.399	1.00	70.09	C
ATOM	3300	CB	ALA	A	430	68.643	13.545	15.703	1.00	70.09	C
ATOM	3301	C	ALA	A	430	70.757	12.249	15.813	1.00	69.03	C

260/396

Figure 3A-60

ATOM	3302	O	ALA	A	430	70.803	12.065	14.617	1.00	68.80	O
ATOM	3303	N	ASP	A	431	71.424	11.539	16.690	1.00	68.13	N
ATOM	3304	CA	ASP	A	431	72.114	10.330	16.321	1.00	67.58	C
ATOM	3305	CB	ASP	A	431	72.579	9.606	17.603	1.00	68.14	C
ATOM	3306	CG	ASP	A	431	72.760	10.582	18.817	1.00	70.28	C
ATOM	3307	OD1	ASP	A	431	72.264	10.295	19.940	1.00	71.36	O
ATOM	3308	OD2	ASP	A	431	73.377	11.677	18.741	1.00	73.13	O
ATOM	3309	C	ASP	A	431	71.158	9.485	15.463	1.00	66.39	C
ATOM	3310	O	ASP	A	431	69.967	9.389	15.780	1.00	66.03	O
ATOM	3311	N	ASN	A	432	71.668	8.950	14.345	1.00	65.02	N
ATOM	3312	CA	ASN	A	432	70.973	7.940	13.537	1.00	63.24	C
ATOM	3313	CB	ASN	A	432	71.982	7.152	12.689	1.00	63.32	C
ATOM	3314	CG	ASN	A	432	72.503	5.887	13.413	1.00	63.38	C
ATOM	3315	OD1	ASN	A	432	72.323	4.749	12.939	1.00	62.25	O
ATOM	3316	ND2	ASN	A	432	73.144	6.092	14.571	1.00	62.72	N
ATOM	3317	C	ASN	A	432	70.279	6.964	14.469	1.00	61.91	C
ATOM	3318	O	ASN	A	432	69.624	6.006	14.030	1.00	61.45	O
ATOM	3319	N	GLU	A	433	70.427	7.263	15.759	1.00	60.38	N
ATOM	3320	CA	GLU	A	433	70.176	6.341	16.849	1.00	59.45	C
ATOM	3321	CB	GLU	A	433	71.520	5.932	17.438	1.00	59.98	C
ATOM	3322	CG	GLU	A	433	71.723	4.428	17.539	1.00	59.30	C
ATOM	3323	CD	GLU	A	433	72.653	4.040	18.666	1.00	57.52	C
ATOM	3324	OE1	GLU	A	433	72.364	4.397	19.843	1.00	55.07	O
ATOM	3325	OE2	GLU	A	433	73.662	3.367	18.357	1.00	57.53	O
ATOM	3326	C	GLU	A	433	69.229	6.826	17.971	1.00	58.66	C
ATOM	3327	O	GLU	A	433	68.830	6.029	18.843	1.00	58.06	O
ATOM	3328	N	THR	A	434	68.894	8.120	17.965	1.00	57.84	N
ATOM	3329	CA	THR	A	434	67.727	8.616	18.713	1.00	57.25	C
ATOM	3330	CB	THR	A	434	67.709	10.131	18.799	1.00	57.31	C
ATOM	3331	OG1	THR	A	434	67.956	10.665	17.486	1.00	58.36	O
ATOM	3332	CG2	THR	A	434	68.844	10.644	19.678	1.00	56.50	C
ATOM	3333	C	THR	A	434	66.497	8.176	17.929	1.00	56.56	C
ATOM	3334	O	THR	A	434	65.417	7.954	18.504	1.00	56.35	O
ATOM	3335	N	GLU	A	435	66.686	8.096	16.608	1.00	55.53	N
ATOM	3336	CA	GLU	A	435	65.810	7.360	15.691	1.00	55.02	C
ATOM	3337	CB	GLU	A	435	66.454	7.251	14.283	1.00	55.91	C
ATOM	3338	CG	GLU	A	435	66.179	8.414	13.302	1.00	60.61	C
ATOM	3339	CD	GLU	A	435	66.218	9.839	13.924	1.00	66.40	C
ATOM	3340	OE1	GLU	A	435	65.203	10.282	14.556	1.00	67.53	O
ATOM	3341	OE2	GLU	A	435	67.256	10.547	13.758	1.00	68.18	O
ATOM	3342	C	GLU	A	435	65.383	5.979	16.263	1.00	53.21	C
ATOM	3343	O	GLU	A	435	64.402	5.899	17.024	1.00	53.89	O
ATOM	3344	N	ILE	A	436	66.104	4.906	15.951	1.00	50.24	N
ATOM	3345	CA	ILE	A	436	65.622	3.579	16.310	1.00	47.74	C
ATOM	3346	CB	ILE	A	436	66.711	2.558	16.034	1.00	47.50	C
ATOM	3347	CG1	ILE	A	436	66.968	2.482	14.519	1.00	46.95	C
ATOM	3348	CD1	ILE	A	436	67.285	3.832	13.784	1.00	45.05	C
ATOM	3349	CG2	ILE	A	436	66.341	1.195	16.612	1.00	45.84	C
ATOM	3350	C	ILE	A	436	65.090	3.535	17.751	1.00	46.97	C
ATOM	3351	O	ILE	A	436	64.167	2.789	18.081	1.00	46.21	O
ATOM	3352	N	ASN	A	437	65.663	4.393	18.583	1.00	46.32	N
ATOM	3353	CA	ASN	A	437	65.240	4.575	19.965	1.00	45.85	C
ATOM	3354	CB	ASN	A	437	65.995	5.766	20.587	1.00	46.33	C
ATOM	3355	CG	ASN	A	437	67.088	5.341	21.560	1.00	45.51	C
ATOM	3356	OD1	ASN	A	437	67.665	4.238	21.425	1.00	44.10	O
ATOM	3357	ND2	ASN	A	437	67.381	6.217	22.543	1.00	40.79	N

261/396

Figure 3A-61

ATOM	3358	C	ASN	A	437	63.768	4.877	20.034	1.00	44.94	C
ATOM	3359	O	ASN	A	437	62.941	4.015	20.341	1.00	44.80	O
ATOM	3360	N	PHE	A	438	63.469	6.130	19.730	1.00	43.79	N
ATOM	3361	CA	PHE	A	438	62.111	6.646	19.723	1.00	43.12	C
ATOM	3362	CB	PHE	A	438	62.146	8.049	19.144	1.00	43.43	C
ATOM	3363	CG	PHE	A	438	60.980	8.385	18.310	1.00	45.45	C
ATOM	3364	CD1	PHE	A	438	60.161	9.453	18.667	1.00	47.70	C
ATOM	3365	CE1	PHE	A	438	59.076	9.814	17.881	1.00	49.56	C
ATOM	3366	CZ	PHE	A	438	58.796	9.080	16.718	1.00	50.82	C
ATOM	3367	CE2	PHE	A	438	59.618	7.997	16.357	1.00	49.65	C
ATOM	3368	CD2	PHE	A	438	60.708	7.671	17.147	1.00	46.74	C
ATOM	3369	C	PHE	A	438	61.112	5.741	18.974	1.00	41.69	C
ATOM	3370	O	PHE	A	438	60.145	5.234	19.561	1.00	40.94	O
ATOM	3371	N	LEU	A	439	61.365	5.516	17.691	1.00	39.85	N
ATOM	3372	CA	LEU	A	439	60.579	4.534	16.981	1.00	38.72	C
ATOM	3373	CB	LEU	A	439	61.195	4.225	15.643	1.00	38.67	C
ATOM	3374	CG	LEU	A	439	60.328	5.005	14.667	1.00	39.84	C
ATOM	3375	CD1	LEU	A	439	61.182	6.063	13.959	1.00	40.82	C
ATOM	3376	CD2	LEU	A	439	59.613	4.083	13.696	1.00	39.45	C
ATOM	3377	C	LEU	A	439	60.341	3.257	17.787	1.00	37.63	C
ATOM	3378	O	LEU	A	439	59.203	2.765	17.847	1.00	37.56	O
ATOM	3379	N	LEU	A	440	61.382	2.722	18.430	1.00	35.90	N
ATOM	3380	CA	LEU	A	440	61.141	1.528	19.219	1.00	34.03	C
ATOM	3381	CB	LEU	A	440	62.411	0.869	19.778	1.00	33.53	C
ATOM	3382	CG	LEU	A	440	62.345	-0.380	20.709	1.00	31.68	C
ATOM	3383	CD1	LEU	A	440	61.897	0.029	22.095	1.00	31.38	C
ATOM	3384	CD2	LEU	A	440	61.520	-1.576	20.228	1.00	27.90	C
ATOM	3385	C	LEU	A	440	60.131	1.852	20.297	1.00	33.15	C
ATOM	3386	O	LEU	A	440	59.358	0.993	20.680	1.00	32.86	O
ATOM	3387	N	LYS	A	441	60.079	3.091	20.759	1.00	32.23	N
ATOM	3388	CA	LYS	A	441	58.986	3.390	21.687	1.00	32.17	C
ATOM	3389	CB	LYS	A	441	59.137	4.751	22.351	1.00	32.10	C
ATOM	3390	CG	LYS	A	441	58.293	4.898	23.561	1.00	30.51	C
ATOM	3391	CD	LYS	A	441	58.240	6.346	23.925	1.00	31.68	C
ATOM	3392	CE	LYS	A	441	57.863	6.460	25.386	1.00	35.31	C
ATOM	3393	NZ	LYS	A	441	57.468	5.108	25.967	1.00	36.76	N
ATOM	3394	C	LYS	A	441	57.612	3.269	20.974	1.00	31.92	C
ATOM	3395	O	LYS	A	441	56.784	2.380	21.315	1.00	31.53	O
ATOM	3396	N	GLN	A	442	57.388	4.143	19.986	1.00	30.36	N
ATOM	3397	CA	GLN	A	442	56.191	4.060	19.173	1.00	29.00	C
ATOM	3398	CB	GLN	A	442	56.446	4.636	17.784	1.00	28.93	C
ATOM	3399	CG	GLN	A	442	56.697	6.103	17.783	1.00	29.49	C
ATOM	3400	CD	GLN	A	442	55.814	6.849	18.767	1.00	31.71	C
ATOM	3401	OE1	GLN	A	442	55.313	7.919	18.436	1.00	32.86	O
ATOM	3402	NE2	GLN	A	442	55.624	6.295	19.984	1.00	31.56	N
ATOM	3403	C	GLN	A	442	55.720	2.615	19.085	1.00	28.17	C
ATOM	3404	O	GLN	A	442	54.737	2.238	19.705	1.00	27.35	O
ATOM	3405	N	ALA	A	443	56.471	1.801	18.356	1.00	27.57	N
ATOM	3406	CA	ALA	A	443	56.060	0.447	18.046	1.00	26.96	C
ATOM	3407	CB	ALA	A	443	57.261	-0.364	17.715	1.00	27.05	C
ATOM	3408	C	ALA	A	443	55.360	-0.149	19.246	1.00	26.61	C
ATOM	3409	O	ALA	A	443	54.446	-0.991	19.126	1.00	25.68	O
ATOM	3410	N	LEU	A	444	55.806	0.313	20.413	1.00	26.33	N
ATOM	3411	CA	LEU	A	444	55.473	-0.361	21.655	1.00	26.36	C
ATOM	3412	CB	LEU	A	444	56.382	0.091	22.812	1.00	25.82	C
ATOM	3413	CG	LEU	A	444	57.275	-0.948	23.539	1.00	22.24	C

262/396

Figure 3A-62

ATOM	3414	CD1	LEU	A	444	57.283	-2.412	22.967	1.00	10.64	C
ATOM	3415	CD2	LEU	A	444	58.670	-0.319	23.675	1.00	20.20	C
ATOM	3416	C	LEU	A	444	54.008	-0.117	21.936	1.00	26.95	C
ATOM	3417	O	LEU	A	444	53.269	-1.057	22.332	1.00	26.99	O
ATOM	3418	N	THR	A	445	53.623	1.147	21.674	1.00	27.25	N
ATOM	3419	CA	THR	A	445	52.235	1.673	21.630	1.00	26.67	C
ATOM	3420	CB	THR	A	445	52.361	3.180	21.840	1.00	25.99	C
ATOM	3421	OG1	THR	A	445	52.507	3.444	23.241	1.00	25.72	O
ATOM	3422	CG2	THR	A	445	51.126	3.892	21.485	1.00	27.71	C
ATOM	3423	C	THR	A	445	51.470	1.293	20.297	1.00	26.61	C
ATOM	3424	O	THR	A	445	50.730	0.257	20.214	1.00	26.15	O
ATOM	3425	N	ILE	A	446	51.710	2.083	19.250	1.00	26.00	N
ATOM	3426	CA	ILE	A	446	51.105	1.851	17.954	1.00	26.10	C
ATOM	3427	CB	ILE	A	446	51.720	2.811	16.945	1.00	26.07	C
ATOM	3428	CG1	ILE	A	446	51.201	4.213	17.204	1.00	28.01	C
ATOM	3429	CD1	ILE	A	446	52.247	5.192	17.779	1.00	31.38	C
ATOM	3430	CG2	ILE	A	446	51.321	2.470	15.548	1.00	26.57	C
ATOM	3431	C	ILE	A	446	51.097	0.385	17.434	1.00	26.18	C
ATOM	3432	O	ILE	A	446	50.172	0.030	16.721	1.00	26.96	O
ATOM	3433	N	VAL	A	447	52.089	-0.458	17.757	1.00	25.95	N
ATOM	3434	CA	VAL	A	447	52.152	-1.810	17.167	1.00	25.17	C
ATOM	3435	CB	VAL	A	447	53.541	-2.240	16.605	1.00	25.12	C
ATOM	3436	CG1	VAL	A	447	53.396	-3.306	15.515	1.00	23.69	C
ATOM	3437	CG2	VAL	A	447	54.319	-1.087	16.093	1.00	24.72	C
ATOM	3438	C	VAL	A	447	51.881	-2.801	18.214	1.00	25.41	C
ATOM	3439	O	VAL	A	447	51.428	-3.906	17.908	1.00	25.02	O
ATOM	3440	N	GLY	A	448	52.219	-2.435	19.445	1.00	25.82	N
ATOM	3441	CA	GLY	A	448	52.006	-3.330	20.566	1.00	27.18	C
ATOM	3442	C	GLY	A	448	50.580	-3.853	20.534	1.00	28.08	C
ATOM	3443	O	GLY	A	448	50.314	-5.068	20.483	1.00	27.50	O
ATOM	3444	N	THR	A	449	49.666	-2.884	20.463	1.00	29.35	N
ATOM	3445	CA	THR	A	449	48.218	-3.079	20.625	1.00	29.64	C
ATOM	3446	CB	THR	A	449	47.574	-1.704	20.870	1.00	29.95	C
ATOM	3447	OG1	THR	A	449	46.263	-1.874	21.425	1.00	31.83	O
ATOM	3448	CG2	THR	A	449	47.348	-0.961	19.536	1.00	30.04	C
ATOM	3449	C	THR	A	449	47.496	-3.773	19.481	1.00	29.05	C
ATOM	3450	O	THR	A	449	46.537	-4.486	19.715	1.00	28.44	O
ATOM	3451	N	LEU	A	450	47.964	-3.549	18.253	1.00	29.22	N
ATOM	3452	CA	LEU	A	450	47.228	-3.964	17.068	1.00	29.38	C
ATOM	3453	CB	LEU	A	450	48.035	-3.844	15.767	1.00	29.21	C
ATOM	3454	CG	LEU	A	450	47.534	-2.679	14.883	1.00	29.64	C
ATOM	3455	CD1	LEU	A	450	48.672	-1.854	14.273	1.00	29.59	C
ATOM	3456	CD2	LEU	A	450	46.570	-3.144	13.773	1.00	30.05	C
ATOM	3457	C	LEU	A	450	46.627	-5.320	17.250	1.00	29.64	C
ATOM	3458	O	LEU	A	450	45.420	-5.438	17.233	1.00	29.43	O
ATOM	3459	N	PRO	A	451	47.431	-6.331	17.530	1.00	30.73	N
ATOM	3460	CA	PRO	A	451	46.900	-7.696	17.577	1.00	31.61	C
ATOM	3461	CB	PRO	A	451	48.149	-8.573	17.354	1.00	31.36	C
ATOM	3462	CG	PRO	A	451	49.309	-7.716	17.735	1.00	31.68	C
ATOM	3463	CD	PRO	A	451	48.855	-6.286	17.913	1.00	31.07	C
ATOM	3464	C	PRO	A	451	46.133	-7.998	18.898	1.00	32.16	C
ATOM	3465	O	PRO	A	451	45.164	-8.754	18.839	1.00	31.54	O
ATOM	3466	N	PHE	A	452	46.545	-7.411	20.029	1.00	33.12	N
ATOM	3467	CA	PHE	A	452	45.655	-7.301	21.187	1.00	34.66	C
ATOM	3468	CB	PHE	A	452	46.236	-6.433	22.342	1.00	34.61	C
ATOM	3469	CG	PHE	A	452	45.330	-6.386	23.571	1.00	36.80	C

263/396

Figure 3A-63

ATOM	3470	CD1	PHE	A	452	44.552	-5.254	23.851	1.00	40.00	C
ATOM	3471	CE1	PHE	A	452	43.661	-5.213	24.982	1.00	39.81	C
ATOM	3472	CZ	PHE	A	452	43.554	-6.324	25.812	1.00	39.93	C
ATOM	3473	CE2	PHE	A	452	44.312	-7.483	25.531	1.00	39.55	C
ATOM	3474	CD2	PHE	A	452	45.185	-7.509	24.410	1.00	38.56	C
ATOM	3475	C	PHE	A	452	44.311	-6.690	20.752	1.00	35.36	C
ATOM	3476	O	PHE	A	452	43.233	-7.311	20.876	1.00	35.99	O
ATOM	3477	N	THR	A	453	44.378	-5.453	20.267	1.00	35.47	N
ATOM	3478	CA	THR	A	453	43.198	-4.749	19.871	1.00	35.27	C
ATOM	3479	CB	THR	A	453	43.596	-3.556	19.119	1.00	34.87	C
ATOM	3480	OG1	THR	A	453	44.493	-2.820	19.938	1.00	34.98	O
ATOM	3481	CG2	THR	A	453	42.446	-2.633	19.012	1.00	36.05	C
ATOM	3482	C	THR	A	453	42.352	-5.671	19.032	1.00	35.88	C
ATOM	3483	O	THR	A	453	41.197	-5.889	19.366	1.00	36.95	O
ATOM	3484	N	TYR	A	454	42.933	-6.259	17.984	1.00	35.90	N
ATOM	3485	CA	TYR	A	454	42.221	-7.207	17.126	1.00	35.62	C
ATOM	3486	CB	TYR	A	454	43.182	-7.826	16.103	1.00	36.27	C
ATOM	3487	CG	TYR	A	454	42.569	-8.875	15.175	1.00	37.75	C
ATOM	3488	CD1	TYR	A	454	42.554	-10.225	15.528	1.00	39.32	C
ATOM	3489	CE1	TYR	A	454	42.021	-11.160	14.711	1.00	39.72	C
ATOM	3490	CZ	TYR	A	454	41.499	-10.759	13.501	1.00	41.79	C
ATOM	3491	OH	TYR	A	454	40.959	-11.697	12.671	1.00	47.67	O
ATOM	3492	CE2	TYR	A	454	41.503	-9.447	13.107	1.00	38.93	C
ATOM	3493	CD2	TYR	A	454	42.040	-8.514	13.939	1.00	38.08	C
ATOM	3494	C	TYR	A	454	41.656	-8.305	17.967	1.00	34.93	C
ATOM	3495	O	TYR	A	454	40.498	-8.313	18.308	1.00	34.49	O
ATOM	3496	N	MET	A	455	42.538	-9.213	18.328	1.00	35.17	N
ATOM	3497	CA	MET	A	455	42.195	-10.439	19.020	1.00	35.21	C
ATOM	3498	CB	MET	A	455	43.357	-10.846	19.963	1.00	35.05	C
ATOM	3499	CG	MET	A	455	43.239	-12.189	20.607	1.00	36.36	C
ATOM	3500	SD	MET	A	455	42.030	-12.147	21.983	1.00	42.95	S
ATOM	3501	CE	MET	A	455	42.188	-13.757	22.764	1.00	41.31	C
ATOM	3502	C	MET	A	455	40.869	-10.263	19.738	1.00	35.03	C
ATOM	3503	O	MET	A	455	39.931	-11.013	19.486	1.00	34.51	O
ATOM	3504	N	LEU	A	456	40.789	-9.228	20.575	1.00	35.26	N
ATOM	3505	CA	LEU	A	456	39.773	-9.159	21.595	1.00	36.07	C
ATOM	3506	CB	LEU	A	456	40.040	-7.983	22.527	1.00	35.61	C
ATOM	3507	CG	LEU	A	456	38.923	-7.550	23.490	1.00	35.04	C
ATOM	3508	CD1	LEU	A	456	39.262	-7.832	24.911	1.00	33.99	C
ATOM	3509	CD2	LEU	A	456	38.620	-6.068	23.351	1.00	34.25	C
ATOM	3510	C	LEU	A	456	38.364	-9.145	20.992	1.00	37.69	C
ATOM	3511	O	LEU	A	456	37.523	-9.948	21.424	1.00	37.90	O
ATOM	3512	N	GLU	A	457	38.111	-8.275	19.990	1.00	38.94	N
ATOM	3513	CA	GLU	A	457	36.805	-8.232	19.285	1.00	39.95	C
ATOM	3514	CB	GLU	A	457	36.714	-7.133	18.210	1.00	39.72	C
ATOM	3515	CG	GLU	A	457	36.989	-5.708	18.697	1.00	42.05	C
ATOM	3516	CD	GLU	A	457	35.759	-4.900	19.196	1.00	43.33	C
ATOM	3517	OE1	GLU	A	457	35.159	-4.167	18.375	1.00	43.08	O
ATOM	3518	OE2	GLU	A	457	35.427	-4.921	20.420	1.00	42.15	O
ATOM	3519	C	GLU	A	457	36.585	-9.560	18.629	1.00	40.41	C
ATOM	3520	O	GLU	A	457	35.528	-10.142	18.742	1.00	40.13	O
ATOM	3521	N	LYS	A	458	37.617	-10.038	17.949	1.00	41.92	N
ATOM	3522	CA	LYS	A	458	37.606	-11.364	17.390	1.00	43.51	C
ATOM	3523	CB	LYS	A	458	39.024	-11.855	17.026	1.00	43.59	C
ATOM	3524	CG	LYS	A	458	39.072	-13.275	16.334	1.00	44.56	C
ATOM	3525	CD	LYS	A	458	38.245	-13.366	14.987	1.00	45.01	C

264/396

Figure 3A-64

ATOM	3526	CE	LYS	A	458	37.443	-14.683	14.921	1.00	44.86	C
ATOM	3527	NZ	LYS	A	458	36.366	-14.798	13.881	1.00	44.57	N
ATOM	3528	C	LYS	A	458	36.992	-12.243	18.453	1.00	44.37	C
ATOM	3529	O	LYS	A	458	36.313	-13.221	18.147	1.00	44.82	O
ATOM	3530	N	TRP	A	459	37.205	-11.889	19.711	1.00	45.15	N
ATOM	3531	CA	TRP	A	459	36.610	-12.687	20.766	1.00	45.99	C
ATOM	3532	CB	TRP	A	459	37.494	-12.723	22.012	1.00	46.29	C
ATOM	3533	CG	TRP	A	459	37.114	-13.835	22.937	1.00	46.75	C
ATOM	3534	CD1	TRP	A	459	37.741	-15.048	23.093	1.00	45.42	C
ATOM	3535	NE1	TRP	A	459	37.101	-15.784	24.057	1.00	45.96	N
ATOM	3536	CE2	TRP	A	459	36.025	-15.067	24.515	1.00	47.55	C
ATOM	3537	CD2	TRP	A	459	36.016	-13.829	23.833	1.00	47.04	C
ATOM	3538	CE3	TRP	A	459	35.018	-12.893	24.138	1.00	46.31	C
ATOM	3539	CZ3	TRP	A	459	34.082	-13.208	25.067	1.00	48.03	C
ATOM	3540	CH2	TRP	A	459	34.103	-14.460	25.731	1.00	50.37	C
ATOM	3541	CZ2	TRP	A	459	35.066	-15.400	25.462	1.00	49.10	C
ATOM	3542	C	TRP	A	459	35.181	-12.241	21.076	1.00	46.29	C
ATOM	3543	O	TRP	A	459	34.275	-13.100	21.101	1.00	46.33	O
ATOM	3544	N	ARG	A	460	34.996	-10.919	21.295	1.00	46.20	N
ATOM	3545	CA	ARG	A	460	33.669	-10.294	21.538	1.00	45.86	C
ATOM	3546	CB	ARG	A	460	33.779	-8.770	21.754	1.00	45.55	C
ATOM	3547	CG	ARG	A	460	32.662	-8.102	22.612	1.00	43.95	C
ATOM	3548	CD	ARG	A	460	33.147	-7.424	23.927	1.00	42.05	C
ATOM	3549	NE	ARG	A	460	33.470	-5.970	23.929	1.00	41.08	N
ATOM	3550	CZ	ARG	A	460	34.419	-5.348	23.180	1.00	40.56	C
ATOM	3551	NH1	ARG	A	460	35.148	-6.016	22.294	1.00	39.63	N
ATOM	3552	NH2	ARG	A	460	34.632	-4.036	23.291	1.00	38.40	N
ATOM	3553	C	ARG	A	460	32.682	-10.642	20.408	1.00	46.14	C
ATOM	3554	O	ARG	A	460	31.594	-11.172	20.677	1.00	46.00	O
ATOM	3555	N	TRP	A	461	33.090	-10.393	19.157	1.00	46.31	N
ATOM	3556	CA	TRP	A	461	32.319	-10.805	17.986	1.00	46.67	C
ATOM	3557	CB	TRP	A	461	33.127	-10.671	16.704	1.00	46.63	C
ATOM	3558	CG	TRP	A	461	33.234	-9.300	16.167	1.00	47.40	C
ATOM	3559	CD1	TRP	A	461	32.358	-8.274	16.337	1.00	48.78	C
ATOM	3560	NE1	TRP	A	461	32.805	-7.153	15.677	1.00	48.67	N
ATOM	3561	CE2	TRP	A	461	33.990	-7.448	15.066	1.00	47.19	C
ATOM	3562	CD2	TRP	A	461	34.289	-8.792	15.356	1.00	47.14	C
ATOM	3563	CE3	TRP	A	461	35.468	-9.339	14.848	1.00	46.90	C
ATOM	3564	CZ3	TRP	A	461	36.284	-8.552	14.085	1.00	47.34	C
ATOM	3565	CH2	TRP	A	461	35.959	-7.220	13.817	1.00	48.03	C
ATOM	3566	CZ2	TRP	A	461	34.813	-6.652	14.299	1.00	47.61	C
ATOM	3567	C	TRP	A	461	31.864	-12.245	18.070	1.00	46.89	C
ATOM	3568	O	TRP	A	461	30.762	-12.566	17.650	1.00	47.32	O
ATOM	3569	N	MET	A	462	32.708	-13.110	18.612	1.00	47.11	N
ATOM	3570	CA	MET	A	462	32.525	-14.545	18.431	1.00	47.63	C
ATOM	3571	CB	MET	A	462	33.819	-15.281	18.769	1.00	48.19	C
ATOM	3572	CG	MET	A	462	34.973	-15.075	17.791	1.00	49.15	C
ATOM	3573	SD	MET	A	462	35.457	-16.530	16.835	1.00	51.57	S
ATOM	3574	CE	MET	A	462	35.596	-17.952	18.140	1.00	49.78	C
ATOM	3575	C	MET	A	462	31.422	-15.090	19.302	1.00	47.54	C
ATOM	3576	O	MET	A	462	30.828	-16.128	19.013	1.00	47.22	O
ATOM	3577	N	VAL	A	463	31.170	-14.360	20.378	1.00	47.69	N
ATOM	3578	CA	VAL	A	463	30.283	-14.759	21.460	1.00	47.89	C
ATOM	3579	CB	VAL	A	463	30.756	-13.954	22.673	1.00	47.52	C
ATOM	3580	CG1	VAL	A	463	30.206	-14.484	23.957	1.00	48.05	C
ATOM	3581	CG2	VAL	A	463	32.253	-14.020	22.717	1.00	46.63	C

265/396

Figure 3A-65

ATOM	3582	C	VAL A 463	28.814	-14.457	21.055	1.00	48.51	C
ATOM	3583	O	VAL A 463	27.882	-15.306	21.102	1.00	47.62	O
ATOM	3584	N	PHE A 464	28.662	-13.202	20.660	1.00	49.26	N
ATOM	3585	CA	PHE A 464	27.559	-12.696	19.890	1.00	49.79	C
ATOM	3586	CB	PHE A 464	27.913	-11.282	19.449	1.00	49.39	C
ATOM	3587	CG	PHE A 464	28.310	-10.338	20.593	1.00	47.43	C
ATOM	3588	CD1	PHE A 464	28.698	-9.033	20.321	1.00	44.06	C
ATOM	3589	CE1	PHE A 464	29.021	-8.165	21.317	1.00	42.83	C
ATOM	3590	CZ	PHE A 464	28.978	-8.556	22.614	1.00	42.90	C
ATOM	3591	CE2	PHE A 464	28.613	-9.840	22.925	1.00	45.40	C
ATOM	3592	CD2	PHE A 464	28.273	-10.737	21.917	1.00	46.59	C
ATOM	3593	C	PHE A 464	27.280	-13.574	18.669	1.00	50.97	C
ATOM	3594	O	PHE A 464	26.161	-13.972	18.457	1.00	51.49	O
ATOM	3595	N	LYS A 465	28.280	-13.894	17.868	1.00	52.43	N
ATOM	3596	CA	LYS A 465	28.040	-14.758	16.715	1.00	54.54	C
ATOM	3597	CB	LYS A 465	29.287	-14.833	15.804	1.00	54.97	C
ATOM	3598	CG	LYS A 465	29.034	-15.193	14.311	1.00	55.80	C
ATOM	3599	CD	LYS A 465	30.293	-15.008	13.407	1.00	56.99	C
ATOM	3600	CE	LYS A 465	30.410	-13.578	12.811	1.00	58.13	C
ATOM	3601	NZ	LYS A 465	31.122	-13.488	11.468	1.00	58.53	N
ATOM	3602	C	LYS A 465	27.589	-16.169	17.111	1.00	55.89	C
ATOM	3603	O	LYS A 465	26.974	-16.858	16.294	1.00	56.42	O
ATOM	3604	N	GLY A 466	27.907	-16.608	18.338	1.00	57.33	N
ATOM	3605	CA	GLY A 466	27.627	-17.981	18.788	1.00	58.68	C
ATOM	3606	C	GLY A 466	28.768	-19.019	18.748	1.00	59.59	C
ATOM	3607	O	GLY A 466	28.687	-20.079	19.392	1.00	59.20	O
ATOM	3608	N	GLU A 467	29.826	-18.710	17.995	1.00	60.63	N
ATOM	3609	CA	GLU A 467	30.938	-19.628	17.728	1.00	61.95	C
ATOM	3610	CB	GLU A 467	32.036	-18.935	16.883	1.00	62.59	C
ATOM	3611	CG	GLU A 467	31.549	-18.241	15.596	1.00	66.48	C
ATOM	3612	CD	GLU A 467	32.615	-17.375	14.878	1.00	70.96	C
ATOM	3613	OE1	GLU A 467	32.601	-16.123	15.049	1.00	73.02	O
ATOM	3614	OE2	GLU A 467	33.460	-17.924	14.113	1.00	72.05	O
ATOM	3615	C	GLU A 467	31.546	-20.202	19.004	1.00	61.89	C
ATOM	3616	O	GLU A 467	32.402	-21.081	18.951	1.00	61.88	O
ATOM	3617	N	ILE A 468	31.102	-19.694	20.146	1.00	62.27	N
ATOM	3618	CA	ILE A 468	31.667	-20.071	21.441	1.00	62.82	C
ATOM	3619	CB	ILE A 468	32.970	-19.246	21.784	1.00	62.54	C
ATOM	3620	CG1	ILE A 468	33.066	-17.947	21.014	1.00	61.43	C
ATOM	3621	CD1	ILE A 468	34.176	-17.129	21.511	1.00	61.50	C
ATOM	3622	CG2	ILE A 468	34.199	-20.006	21.443	1.00	63.07	C
ATOM	3623	C	ILE A 468	30.628	-19.955	22.576	1.00	63.43	C
ATOM	3624	O	ILE A 468	30.078	-18.872	22.837	1.00	63.84	O
ATOM	3625	N	PRO A 469	30.334	-21.067	23.237	1.00	63.83	N
ATOM	3626	CA	PRO A 469	29.336	-21.069	24.319	1.00	64.06	C
ATOM	3627	CB	PRO A 469	28.580	-22.377	24.083	1.00	64.22	C
ATOM	3628	CG	PRO A 469	29.581	-23.231	23.184	1.00	64.79	C
ATOM	3629	CD	PRO A 469	30.855	-22.416	22.958	1.00	63.79	C
ATOM	3630	C	PRO A 469	29.911	-21.038	25.735	1.00	64.12	C
ATOM	3631	O	PRO A 469	30.758	-21.849	26.107	1.00	63.91	O
ATOM	3632	N	LYS A 470	29.424	-20.077	26.508	1.00	64.39	N
ATOM	3633	CA	LYS A 470	29.666	-19.990	27.935	1.00	64.57	C
ATOM	3634	CB	LYS A 470	28.379	-20.290	28.705	1.00	64.71	C
ATOM	3635	CG	LYS A 470	27.082	-20.029	27.920	1.00	65.33	C
ATOM	3636	CD	LYS A 470	26.107	-19.166	28.731	1.00	66.86	C
ATOM	3637	CE	LYS A 470	25.488	-18.035	27.902	1.00	67.09	C

266/396

Figure 3A-66

ATOM	3638	NZ	LYS	A	470	25.964	-16.665	28.285	1.00	65.98	N
ATOM	3639	C	LYS	A	470	30.784	-20.916	28.366	1.00	64.74	C
ATOM	3640	O	LYS	A	470	31.944	-20.523	28.306	1.00	64.78	O
ATOM	3641	N	ASP	A	471	30.420	-22.144	28.755	1.00	65.35	N
ATOM	3642	CA	ASP	A	471	31.333	-23.218	29.241	1.00	66.05	C
ATOM	3643	CB	ASP	A	471	30.581	-24.583	29.337	1.00	66.48	C
ATOM	3644	CG	ASP	A	471	30.573	-25.384	27.989	1.00	67.47	C
ATOM	3645	OD1	ASP	A	471	30.400	-24.756	26.905	1.00	67.14	O
ATOM	3646	OD2	ASP	A	471	30.719	-26.642	27.929	1.00	67.59	O
ATOM	3647	C	ASP	A	471	32.688	-23.414	28.500	1.00	65.83	C
ATOM	3648	O	ASP	A	471	33.518	-24.249	28.918	1.00	65.56	O
ATOM	3649	N	GLN	A	472	32.892	-22.666	27.406	1.00	65.42	N
ATOM	3650	CA	GLN	A	472	34.178	-22.657	26.702	1.00	64.87	C
ATOM	3651	CB	GLN	A	472	34.129	-23.581	25.462	1.00	65.22	C
ATOM	3652	CG	GLN	A	472	33.616	-25.036	25.759	1.00	67.61	C
ATOM	3653	CD	GLN	A	472	34.724	-26.138	25.906	1.00	70.75	C
ATOM	3654	OE1	GLN	A	472	35.374	-26.547	24.907	1.00	71.10	O
ATOM	3655	NE2	GLN	A	472	34.897	-26.640	27.144	1.00	70.48	N
ATOM	3656	C	GLN	A	472	34.800	-21.251	26.404	1.00	63.69	C
ATOM	3657	O	GLN	A	472	35.815	-21.166	25.703	1.00	63.73	O
ATOM	3658	N	TRP	A	473	34.235	-20.180	26.976	1.00	62.19	N
ATOM	3659	CA	TRP	A	473	34.748	-18.807	26.788	1.00	60.94	C
ATOM	3660	CB	TRP	A	473	33.904	-17.819	27.541	1.00	60.81	C
ATOM	3661	CG	TRP	A	473	32.653	-17.505	27.037	1.00	59.44	C
ATOM	3662	CD1	TRP	A	473	32.063	-17.987	25.939	1.00	59.72	C
ATOM	3663	NE1	TRP	A	473	30.809	-17.444	25.803	1.00	60.87	N
ATOM	3664	CE2	TRP	A	473	30.593	-16.593	26.849	1.00	61.13	C
ATOM	3665	CD2	TRP	A	473	31.751	-16.615	27.642	1.00	60.03	C
ATOM	3666	CE3	TRP	A	473	31.799	-15.816	28.794	1.00	61.11	C
ATOM	3667	CZ3	TRP	A	473	30.700	-15.031	29.120	1.00	62.93	C
ATOM	3668	CH2	TRP	A	473	29.554	-15.025	28.301	1.00	64.04	C
ATOM	3669	CZ2	TRP	A	473	29.481	-15.804	27.161	1.00	63.02	C
ATOM	3670	C	TRP	A	473	36.146	-18.505	27.324	1.00	60.31	C
ATOM	3671	O	TRP	A	473	36.911	-17.736	26.718	1.00	59.99	O
ATOM	3672	N	MET	A	474	36.443	-19.013	28.512	1.00	59.46	N
ATOM	3673	CA	MET	A	474	37.718	-18.693	29.103	1.00	59.24	C
ATOM	3674	CB	MET	A	474	37.780	-19.053	30.565	1.00	59.18	C
ATOM	3675	CG	MET	A	474	38.241	-17.891	31.384	1.00	59.29	C
ATOM	3676	SD	MET	A	474	37.534	-16.408	30.678	1.00	60.52	S
ATOM	3677	CE	MET	A	474	38.951	-15.688	29.895	1.00	61.71	C
ATOM	3678	C	MET	A	474	38.801	-19.396	28.360	1.00	59.32	C
ATOM	3679	O	MET	A	474	39.807	-18.784	27.988	1.00	59.11	O
ATOM	3680	N	LYS	A	475	38.571	-20.683	28.128	1.00	59.39	N
ATOM	3681	CA	LYS	A	475	39.432	-21.452	27.254	1.00	59.82	C
ATOM	3682	CB	LYS	A	475	38.916	-22.883	27.095	1.00	60.13	C
ATOM	3683	CG	LYS	A	475	39.683	-23.867	28.007	1.00	62.25	C
ATOM	3684	CD	LYS	A	475	40.768	-24.654	27.244	1.00	64.22	C
ATOM	3685	CE	LYS	A	475	40.199	-25.975	26.639	1.00	64.58	C
ATOM	3686	NZ	LYS	A	475	40.995	-26.494	25.464	1.00	64.31	N
ATOM	3687	C	LYS	A	475	39.744	-20.751	25.892	1.00	59.38	C
ATOM	3688	O	LYS	A	475	40.929	-20.491	25.587	1.00	59.96	O
ATOM	3689	N	LYS	A	476	38.733	-20.411	25.086	1.00	57.97	N
ATOM	3690	CA	LYS	A	476	39.055	-19.808	23.789	1.00	56.52	C
ATOM	3691	CB	LYS	A	476	37.815	-19.379	23.003	1.00	56.69	C
ATOM	3692	CG	LYS	A	476	37.464	-20.330	21.859	1.00	56.91	C
ATOM	3693	CD	LYS	A	476	37.824	-19.829	20.442	1.00	56.03	C

267/396

Figure 3A-67

ATOM	3694	CE	LYS	A	476	37.544	-20.930	19.381	1.00	56.15	C
ATOM	3695	NZ	LYS	A	476	36.799	-22.190	19.837	1.00	54.47	N
ATOM	3696	C	LYS	A	476	40.008	-18.650	23.991	1.00	55.50	C
ATOM	3697	O	LYS	A	476	41.037	-18.567	23.340	1.00	55.01	O
ATOM	3698	N	TRP	A	477	39.678	-17.787	24.939	1.00	54.62	N
ATOM	3699	CA	TRP	A	477	40.483	-16.616	25.221	1.00	54.20	C
ATOM	3700	CB	TRP	A	477	40.025	-16.042	26.537	1.00	53.90	C
ATOM	3701	CG	TRP	A	477	40.604	-14.718	26.829	1.00	52.56	C
ATOM	3702	CD1	TRP	A	477	41.614	-14.439	27.703	1.00	51.48	C
ATOM	3703	NE1	TRP	A	477	41.862	-13.088	27.711	1.00	51.34	N
ATOM	3704	CE2	TRP	A	477	41.004	-12.470	26.836	1.00	50.45	C
ATOM	3705	CD2	TRP	A	477	40.197	-13.469	26.265	1.00	50.48	C
ATOM	3706	CE3	TRP	A	477	39.213	-13.092	25.347	1.00	49.30	C
ATOM	3707	CZ3	TRP	A	477	39.081	-11.777	25.026	1.00	49.14	C
ATOM	3708	CH2	TRP	A	477	39.898	-10.806	25.610	1.00	50.04	C
ATOM	3709	CZ2	TRP	A	477	40.860	-11.128	26.518	1.00	49.60	C
ATOM	3710	C	TRP	A	477	41.996	-16.884	25.293	1.00	54.28	C
ATOM	3711	O	TRP	A	477	42.803	-16.359	24.504	1.00	53.58	O
ATOM	3712	N	TRP	A	478	42.367	-17.707	26.263	1.00	54.53	N
ATOM	3713	CA	TRP	A	478	43.762	-18.021	26.475	1.00	54.69	C
ATOM	3714	CB	TRP	A	478	43.960	-18.700	27.822	1.00	53.80	C
ATOM	3715	CG	TRP	A	478	43.813	-17.675	28.860	1.00	51.91	C
ATOM	3716	CD1	TRP	A	478	42.795	-17.562	29.739	1.00	51.39	C
ATOM	3717	NE1	TRP	A	478	42.969	-16.449	30.530	1.00	51.11	N
ATOM	3718	CE2	TRP	A	478	44.115	-15.797	30.151	1.00	50.04	C
ATOM	3719	CD2	TRP	A	478	44.669	-16.529	29.083	1.00	50.48	C
ATOM	3720	CE3	TRP	A	478	45.870	-16.061	28.501	1.00	49.07	C
ATOM	3721	CZ3	TRP	A	478	46.455	-14.898	28.999	1.00	45.79	C
ATOM	3722	CH2	TRP	A	478	45.868	-14.196	30.061	1.00	46.06	C
ATOM	3723	CZ2	TRP	A	478	44.708	-14.627	30.655	1.00	47.83	C
ATOM	3724	C	TRP	A	478	44.360	-18.779	25.308	1.00	55.68	C
ATOM	3725	O	TRP	A	478	45.539	-18.589	24.991	1.00	56.04	O
ATOM	3726	N	GLU	A	479	43.530	-19.582	24.640	1.00	56.53	N
ATOM	3727	CA	GLU	A	479	43.890	-20.207	23.363	1.00	57.59	C
ATOM	3728	CB	GLU	A	479	42.708	-21.011	22.833	1.00	58.14	C
ATOM	3729	CG	GLU	A	479	43.062	-22.133	21.877	1.00	61.73	C
ATOM	3730	CD	GLU	A	479	42.258	-23.390	22.190	1.00	68.04	C
ATOM	3731	OE1	GLU	A	479	40.991	-23.314	22.071	1.00	68.63	O
ATOM	3732	OE2	GLU	A	479	42.888	-24.443	22.572	1.00	71.04	O
ATOM	3733	C	GLU	A	479	44.333	-19.185	22.295	1.00	57.17	C
ATOM	3734	O	GLU	A	479	45.332	-19.411	21.584	1.00	56.96	O
ATOM	3735	N	MET	A	480	43.589	-18.073	22.205	1.00	56.74	N
ATOM	3736	CA	MET	A	480	43.787	-17.045	21.168	1.00	56.23	C
ATOM	3737	CB	MET	A	480	42.450	-16.423	20.774	1.00	56.14	C
ATOM	3738	CG	MET	A	480	41.291	-17.378	20.720	1.00	55.66	C
ATOM	3739	SD	MET	A	480	39.727	-16.512	20.960	1.00	56.18	S
ATOM	3740	CE	MET	A	480	39.575	-15.625	19.318	1.00	55.85	C
ATOM	3741	C	MET	A	480	44.787	-15.945	21.571	1.00	55.88	C
ATOM	3742	O	MET	A	480	45.512	-15.376	20.731	1.00	55.09	O
ATOM	3743	N	LYS	A	481	44.812	-15.651	22.866	1.00	55.65	N
ATOM	3744	CA	LYS	A	481	45.915	-14.895	23.424	1.00	55.54	C
ATOM	3745	CB	LYS	A	481	45.672	-14.588	24.902	1.00	55.40	C
ATOM	3746	CG	LYS	A	481	44.736	-13.404	25.132	1.00	54.42	C
ATOM	3747	CD	LYS	A	481	45.472	-12.095	25.331	1.00	52.13	C
ATOM	3748	CE	LYS	A	481	44.932	-11.337	26.525	1.00	51.88	C
ATOM	3749	NZ	LYS	A	481	43.666	-10.617	26.217	1.00	51.35	N

268/396

Figure 3A-68

ATOM	3750	C	LYS	A	481	47.222	-15.676	23.201	1.00	55.61	C
ATOM	3751	O	LYS	A	481	48.321	-15.097	23.190	1.00	55.43	O
ATOM	3752	N	ARG	A	482	47.087	-16.989	23.009	1.00	55.36	N
ATOM	3753	CA	ARG	A	482	48.205	-17.791	22.573	1.00	55.54	C
ATOM	3754	CB	ARG	A	482	48.061	-19.237	23.005	1.00	55.63	C
ATOM	3755	CG	ARG	A	482	48.937	-19.532	24.191	1.00	57.27	C
ATOM	3756	CD	ARG	A	482	48.972	-20.989	24.622	1.00	60.21	C
ATOM	3757	NE	ARG	A	482	47.892	-21.338	25.558	1.00	61.09	N
ATOM	3758	CZ	ARG	A	482	48.046	-21.534	26.860	1.00	60.64	C
ATOM	3759	NH1	ARG	A	482	49.250	-21.420	27.424	1.00	60.00	N
ATOM	3760	NH2	ARG	A	482	46.989	-21.858	27.596	1.00	60.55	N
ATOM	3761	C	ARG	A	482	48.467	-17.689	21.073	1.00	55.41	C
ATOM	3762	O	ARG	A	482	49.532	-17.187	20.668	1.00	55.62	O
ATOM	3763	N	GLU	A	483	47.519	-18.153	20.252	1.00	54.89	N
ATOM	3764	CA	GLU	A	483	47.744	-18.232	18.798	1.00	54.35	C
ATOM	3765	CB	GLU	A	483	46.546	-18.868	18.084	1.00	54.82	C
ATOM	3766	CG	GLU	A	483	46.774	-20.302	17.605	1.00	58.51	C
ATOM	3767	CD	GLU	A	483	45.916	-20.707	16.377	1.00	64.61	C
ATOM	3768	OE1	GLU	A	483	44.785	-20.149	16.148	1.00	65.44	O
ATOM	3769	OE2	GLU	A	483	46.377	-21.619	15.625	1.00	66.48	O
ATOM	3770	C	GLU	A	483	48.107	-16.865	18.181	1.00	53.01	C
ATOM	3771	O	GLU	A	483	49.144	-16.752	17.502	1.00	52.50	O
ATOM	3772	N	ILE	A	484	47.281	-15.845	18.495	1.00	51.48	N
ATOM	3773	CA	ILE	A	484	47.290	-14.499	17.883	1.00	49.29	C
ATOM	3774	CB	ILE	A	484	45.831	-13.990	17.658	1.00	48.94	C
ATOM	3775	CG1	ILE	A	484	44.926	-15.084	17.102	1.00	47.10	C
ATOM	3776	CD1	ILE	A	484	43.466	-14.836	17.335	1.00	43.02	C
ATOM	3777	CG2	ILE	A	484	45.796	-12.810	16.723	1.00	48.41	C
ATOM	3778	C	ILE	A	484	48.081	-13.438	18.664	1.00	48.77	C
ATOM	3779	O	ILE	A	484	48.740	-12.607	18.077	1.00	48.66	O
ATOM	3780	N	VAL	A	485	48.039	-13.432	19.980	1.00	48.23	N
ATOM	3781	CA	VAL	A	485	48.779	-12.377	20.662	1.00	48.33	C
ATOM	3782	CB	VAL	A	485	48.103	-11.979	21.941	1.00	48.44	C
ATOM	3783	CG1	VAL	A	485	48.236	-10.479	22.127	1.00	48.93	C
ATOM	3784	CG2	VAL	A	485	46.648	-12.380	21.891	1.00	48.94	C
ATOM	3785	C	VAL	A	485	50.249	-12.675	20.948	1.00	48.38	C
ATOM	3786	O	VAL	A	485	51.099	-11.809	20.891	1.00	47.38	O
ATOM	3787	N	GLY	A	486	50.548	-13.921	21.259	1.00	49.35	N
ATOM	3788	CA	GLY	A	486	51.911	-14.296	21.596	1.00	50.48	C
ATOM	3789	C	GLY	A	486	52.053	-14.226	23.099	1.00	50.88	C
ATOM	3790	O	GLY	A	486	53.187	-14.162	23.672	1.00	50.99	O
ATOM	3791	N	VAL	A	487	50.870	-14.300	23.718	1.00	50.27	N
ATOM	3792	CA	VAL	A	487	50.683	-13.934	25.091	1.00	49.52	C
ATOM	3793	CB	VAL	A	487	49.952	-12.617	25.116	1.00	48.75	C
ATOM	3794	CG1	VAL	A	487	48.909	-12.591	26.162	1.00	48.78	C
ATOM	3795	CG2	VAL	A	487	50.960	-11.528	25.317	1.00	47.26	C
ATOM	3796	C	VAL	A	487	50.027	-15.093	25.846	1.00	49.92	C
ATOM	3797	O	VAL	A	487	49.303	-15.877	25.234	1.00	50.12	O
ATOM	3798	N	VAL	A	488	50.339	-15.236	27.144	1.00	50.03	N
ATOM	3799	CA	VAL	A	488	49.987	-16.433	27.902	1.00	50.28	C
ATOM	3800	CB	VAL	A	488	51.008	-17.565	27.641	1.00	50.49	C
ATOM	3801	CG1	VAL	A	488	51.938	-17.831	28.852	1.00	50.85	C
ATOM	3802	CG2	VAL	A	488	50.279	-18.814	27.261	1.00	51.26	C
ATOM	3803	C	VAL	A	488	49.810	-16.268	29.405	1.00	50.31	C
ATOM	3804	O	VAL	A	488	50.530	-15.503	30.056	1.00	50.22	O
ATOM	3805	N	GLU	A	489	48.889	-17.059	29.949	1.00	50.37	N

269/396

Figure 3A-69

ATOM	3806	CA	GLU	A	489	48.437	-16.926	31.329	1.00	50.50	C
ATOM	3807	CB	GLU	A	489	47.051	-17.535	31.479	1.00	50.38	C
ATOM	3808	CG	GLU	A	489	47.001	-19.038	31.316	1.00	51.35	C
ATOM	3809	CD	GLU	A	489	47.374	-19.504	29.925	1.00	53.19	C
ATOM	3810	OE1	GLU	A	489	46.521	-20.185	29.312	1.00	55.21	O
ATOM	3811	OE2	GLU	A	489	48.502	-19.207	29.454	1.00	51.70	O
ATOM	3812	C	GLU	A	489	49.361	-17.550	32.338	1.00	50.64	C
ATOM	3813	O	GLU	A	489	49.626	-18.741	32.247	1.00	50.43	O
ATOM	3814	N	PRO	A	490	49.855	-16.740	33.287	1.00	51.28	N
ATOM	3815	CA	PRO	A	490	50.608	-17.230	34.471	1.00	51.52	C
ATOM	3816	CB	PRO	A	490	50.946	-15.947	35.263	1.00	51.26	C
ATOM	3817	CG	PRO	A	490	50.784	-14.822	34.290	1.00	51.78	C
ATOM	3818	CD	PRO	A	490	49.803	-15.267	33.238	1.00	51.29	C
ATOM	3819	C	PRO	A	490	49.879	-18.203	35.399	1.00	51.30	C
ATOM	3820	O	PRO	A	490	50.511	-18.674	36.341	1.00	51.74	O
ATOM	3821	N	VAL	A	491	48.616	-18.512	35.134	1.00	50.98	N
ATOM	3822	CA	VAL	A	491	47.794	-19.236	36.080	1.00	51.01	C
ATOM	3823	CB	VAL	A	491	47.341	-18.314	37.248	1.00	51.23	C
ATOM	3824	CG1	VAL	A	491	46.997	-19.132	38.481	1.00	51.47	C
ATOM	3825	CG2	VAL	A	491	48.364	-17.201	37.577	1.00	50.11	C
ATOM	3826	C	VAL	A	491	46.544	-19.726	35.366	1.00	51.50	C
ATOM	3827	O	VAL	A	491	45.786	-18.925	34.836	1.00	51.30	O
ATOM	3828	N	PRO	A	492	46.285	-21.026	35.370	1.00	52.32	N
ATOM	3829	CA	PRO	A	492	45.221	-21.583	34.514	1.00	52.91	C
ATOM	3830	CB	PRO	A	492	45.439	-23.103	34.592	1.00	52.98	C
ATOM	3831	CG	PRO	A	492	46.755	-23.285	35.298	1.00	52.87	C
ATOM	3832	CD	PRO	A	492	46.934	-22.062	36.186	1.00	52.46	C
ATOM	3833	C	PRO	A	492	43.819	-21.202	34.979	1.00	53.45	C
ATOM	3834	O	PRO	A	492	43.250	-21.877	35.852	1.00	53.37	O
ATOM	3835	N	HIS	A	493	43.308	-20.118	34.380	1.00	54.11	N
ATOM	3836	CA	HIS	A	493	41.964	-19.552	34.575	1.00	54.53	C
ATOM	3837	CB	HIS	A	493	41.874	-18.305	33.730	1.00	54.44	C
ATOM	3838	CG	HIS	A	493	42.654	-17.145	34.251	1.00	54.21	C
ATOM	3839	ND1	HIS	A	493	43.228	-17.130	35.503	1.00	53.36	N
ATOM	3840	CE1	HIS	A	493	43.820	-15.965	35.687	1.00	53.35	C
ATOM	3841	NE2	HIS	A	493	43.651	-15.229	34.602	1.00	52.82	N
ATOM	3842	CD2	HIS	A	493	42.930	-15.944	33.687	1.00	53.02	C
ATOM	3843	C	HIS	A	493	40.838	-20.431	34.059	1.00	55.15	C
ATOM	3844	O	HIS	A	493	40.877	-20.845	32.901	1.00	54.88	O
ATOM	3845	N	ASP	A	494	39.818	-20.671	34.884	1.00	56.29	N
ATOM	3846	CA	ASP	A	494	38.685	-21.537	34.497	1.00	57.48	C
ATOM	3847	CB	ASP	A	494	38.471	-22.712	35.507	1.00	58.08	C
ATOM	3848	CG	ASP	A	494	37.361	-22.459	36.549	1.00	58.89	C
ATOM	3849	OD1	ASP	A	494	37.690	-22.503	37.764	1.00	58.85	O
ATOM	3850	OD2	ASP	A	494	36.145	-22.265	36.256	1.00	59.74	O
ATOM	3851	C	ASP	A	494	37.445	-20.707	34.274	1.00	57.76	C
ATOM	3852	O	ASP	A	494	37.425	-19.549	34.677	1.00	57.68	O
ATOM	3853	N	GLU	A	495	36.415	-21.274	33.646	1.00	58.47	N
ATOM	3854	CA	GLU	A	495	35.227	-20.466	33.346	1.00	59.79	C
ATOM	3855	CB	GLU	A	495	34.262	-21.095	32.317	1.00	59.61	C
ATOM	3856	CG	GLU	A	495	34.738	-22.370	31.627	1.00	60.09	C
ATOM	3857	CD	GLU	A	495	35.409	-22.146	30.277	1.00	59.19	C
ATOM	3858	OE1	GLU	A	495	36.189	-23.035	29.866	1.00	58.09	O
ATOM	3859	OE2	GLU	A	495	35.161	-21.099	29.627	1.00	59.47	O
ATOM	3860	C	GLU	A	495	34.524	-20.020	34.630	1.00	60.76	C
ATOM	3861	O	GLU	A	495	33.317	-19.712	34.637	1.00	61.33	O

270/396

Figure 3A-70

ATOM	3862	N	THR	A	496	35.307	-19.987	35.713	1.00	61.54	N
ATOM	3863	CA	THR	A	496	34.980	-19.181	36.885	1.00	61.99	C
ATOM	3864	CB	THR	A	496	35.516	-19.796	38.174	1.00	61.73	C
ATOM	3865	OG1	THR	A	496	34.523	-19.678	39.202	1.00	61.03	O
ATOM	3866	CG2	THR	A	496	36.654	-18.985	38.705	1.00	61.04	C
ATOM	3867	C	THR	A	496	35.469	-17.737	36.707	1.00	62.73	C
ATOM	3868	O	THR	A	496	34.873	-16.808	37.278	1.00	63.54	O
ATOM	3869	N	TYR	A	497	36.515	-17.548	35.896	1.00	62.86	N
ATOM	3870	CA	TYR	A	497	37.012	-16.205	35.514	1.00	62.95	C
ATOM	3871	CB	TYR	A	497	38.513	-16.285	35.215	1.00	63.29	C
ATOM	3872	CG	TYR	A	497	39.317	-16.850	36.377	1.00	65.91	C
ATOM	3873	CD1	TYR	A	497	40.348	-16.108	36.959	1.00	68.34	C
ATOM	3874	CE1	TYR	A	497	41.094	-16.616	38.040	1.00	69.55	C
ATOM	3875	CZ	TYR	A	497	40.804	-17.878	38.553	1.00	69.75	C
ATOM	3876	OH	TYR	A	497	41.540	-18.368	39.624	1.00	69.47	O
ATOM	3877	CE2	TYR	A	497	39.779	-18.637	37.984	1.00	69.31	C
ATOM	3878	CD2	TYR	A	497	39.044	-18.121	36.905	1.00	67.47	C
ATOM	3879	C	TYR	A	497	36.235	-15.636	34.305	1.00	62.08	C
ATOM	3880	O	TYR	A	497	35.578	-16.412	33.604	1.00	62.41	O
ATOM	3881	N	CYS	A	498	36.254	-14.309	34.091	1.00	60.50	N
ATOM	3882	CA	CYS	A	498	35.817	-13.727	32.808	1.00	58.93	C
ATOM	3883	CB	CYS	A	498	34.369	-13.244	32.820	1.00	59.03	C
ATOM	3884	SG	CYS	A	498	33.810	-12.582	31.201	1.00	62.55	S
ATOM	3885	C	CYS	A	498	36.730	-12.601	32.389	1.00	57.41	C
ATOM	3886	O	CYS	A	498	36.315	-11.446	32.302	1.00	56.93	O
ATOM	3887	N	ASP	A	499	37.978	-12.963	32.101	1.00	55.96	N
ATOM	3888	CA	ASP	A	499	39.055	-11.991	31.930	1.00	54.13	C
ATOM	3889	CB	ASP	A	499	40.261	-12.576	31.207	1.00	53.83	C
ATOM	3890	CG	ASP	A	499	40.838	-13.754	31.936	1.00	53.91	C
ATOM	3891	OD1	ASP	A	499	41.207	-14.729	31.253	1.00	53.82	O
ATOM	3892	OD2	ASP	A	499	40.942	-13.803	33.186	1.00	53.55	O
ATOM	3893	C	ASP	A	499	38.550	-10.712	31.301	1.00	53.00	C
ATOM	3894	O	ASP	A	499	38.375	-9.745	32.035	1.00	53.41	O
ATOM	3895	N	PRO	A	500	38.234	-10.704	30.005	1.00	51.52	N
ATOM	3896	CA	PRO	A	500	37.849	-9.469	29.315	1.00	50.57	C
ATOM	3897	CB	PRO	A	500	37.201	-9.983	28.031	1.00	50.54	C
ATOM	3898	CG	PRO	A	500	37.009	-11.408	28.276	1.00	51.33	C
ATOM	3899	CD	PRO	A	500	38.163	-11.848	29.095	1.00	51.42	C
ATOM	3900	C	PRO	A	500	36.855	-8.610	30.134	1.00	49.51	C
ATOM	3901	O	PRO	A	500	37.045	-7.358	30.254	1.00	49.05	O
ATOM	3902	N	ALA	A	501	35.845	-9.269	30.724	1.00	47.43	N
ATOM	3903	CA	ALA	A	501	34.940	-8.579	31.647	1.00	45.51	C
ATOM	3904	CB	ALA	A	501	34.320	-9.543	32.579	1.00	45.50	C
ATOM	3905	C	ALA	A	501	35.696	-7.520	32.431	1.00	43.96	C
ATOM	3906	O	ALA	A	501	35.148	-6.510	32.881	1.00	43.51	O
ATOM	3907	N	SER	A	502	36.982	-7.768	32.576	1.00	42.30	N
ATOM	3908	CA	SER	A	502	37.807	-6.912	33.370	1.00	41.07	C
ATOM	3909	CB	SER	A	502	39.072	-7.639	33.805	1.00	40.81	C
ATOM	3910	OG	SER	A	502	40.055	-7.497	32.802	1.00	41.90	O
ATOM	3911	C	SER	A	502	38.111	-5.616	32.636	1.00	39.75	C
ATOM	3912	O	SER	A	502	37.969	-4.559	33.217	1.00	40.16	O
ATOM	3913	N	LEU	A	503	38.528	-5.650	31.382	1.00	37.89	N
ATOM	3914	CA	LEU	A	503	38.904	-4.369	30.795	1.00	36.14	C
ATOM	3915	CB	LEU	A	503	39.463	-4.529	29.381	1.00	35.85	C
ATOM	3916	CG	LEU	A	503	40.279	-3.421	28.725	1.00	33.26	C
ATOM	3917	CD1	LEU	A	503	40.843	-4.004	27.477	1.00	33.41	C

271/396

Figure 3A-71

ATOM	3918	CD2	LEU	A	503	39.433	-2.282	28.331	1.00	30.80	C
ATOM	3919	C	LEU	A	503	37.634	-3.557	30.750	1.00	35.48	C
ATOM	3920	O	LEU	A	503	36.618	-4.047	30.240	1.00	35.92	O
ATOM	3921	N	PHE	A	504	37.665	-2.363	31.341	1.00	33.86	N
ATOM	3922	CA	PHE	A	504	36.702	-1.311	31.017	1.00	32.45	C
ATOM	3923	CB	PHE	A	504	37.480	-0.023	30.822	1.00	32.26	C
ATOM	3924	CG	PHE	A	504	36.652	1.206	30.806	1.00	31.77	C
ATOM	3925	CD1	PHE	A	504	35.984	1.637	31.941	1.00	32.14	C
ATOM	3926	CE1	PHE	A	504	35.244	2.818	31.936	1.00	30.71	C
ATOM	3927	CZ	PHE	A	504	35.168	3.571	30.793	1.00	31.13	C
ATOM	3928	CE2	PHE	A	504	35.846	3.170	29.660	1.00	31.47	C
ATOM	3929	CD2	PHE	A	504	36.594	1.986	29.675	1.00	32.33	C
ATOM	3930	C	PHE	A	504	35.926	-1.641	29.718	1.00	31.76	C
ATOM	3931	O	PHE	A	504	34.881	-2.301	29.756	1.00	31.39	O
ATOM	3932	N	HIS	A	505	36.455	-1.220	28.572	1.00	30.56	N
ATOM	3933	CA	HIS	A	505	35.769	-1.403	27.304	1.00	29.59	C
ATOM	3934	CB	HIS	A	505	36.749	-1.504	26.167	1.00	28.79	C
ATOM	3935	CG	HIS	A	505	37.697	-0.379	26.110	1.00	26.91	C
ATOM	3936	ND1	HIS	A	505	37.981	0.283	24.942	1.00	24.61	N
ATOM	3937	CE1	HIS	A	505	38.832	1.259	25.194	1.00	24.88	C
ATOM	3938	NE2	HIS	A	505	39.111	1.250	26.482	1.00	27.21	N
ATOM	3939	CD2	HIS	A	505	38.412	0.230	27.080	1.00	26.62	C
ATOM	3940	C	HIS	A	505	34.908	-2.635	27.222	1.00	30.11	C
ATOM	3941	O	HIS	A	505	33.978	-2.653	26.443	1.00	31.31	O
ATOM	3942	N	VAL	A	506	35.214	-3.710	27.932	1.00	29.95	N
ATOM	3943	CA	VAL	A	506	34.274	-4.819	27.870	1.00	29.90	C
ATOM	3944	CB	VAL	A	506	34.897	-6.188	28.174	1.00	29.57	C
ATOM	3945	CG1	VAL	A	506	33.897	-7.268	27.986	1.00	27.94	C
ATOM	3946	CG2	VAL	A	506	36.050	-6.437	27.241	1.00	29.89	C
ATOM	3947	C	VAL	A	506	33.230	-4.366	28.864	1.00	30.47	C
ATOM	3948	O	VAL	A	506	32.347	-3.595	28.501	1.00	30.90	O
ATOM	3949	N	SER	A	507	33.386	-4.752	30.125	1.00	30.76	N
ATOM	3950	CA	SER	A	507	32.512	-4.342	31.220	1.00	30.83	C
ATOM	3951	CB	SER	A	507	33.344	-4.231	32.484	1.00	30.73	C
ATOM	3952	OG	SER	A	507	34.289	-3.192	32.342	1.00	30.63	O
ATOM	3953	C	SER	A	507	31.742	-3.025	31.040	1.00	31.47	C
ATOM	3954	O	SER	A	507	30.659	-2.866	31.596	1.00	32.11	O
ATOM	3955	N	ASN	A	508	32.282	-2.075	30.282	1.00	31.68	N
ATOM	3956	CA	ASN	A	508	31.700	-0.744	30.254	1.00	31.75	C
ATOM	3957	CB	ASN	A	508	32.784	0.273	30.534	1.00	31.42	C
ATOM	3958	CG	ASN	A	508	32.999	0.455	32.007	1.00	32.57	C
ATOM	3959	OD1	ASN	A	508	32.808	1.548	32.508	1.00	36.06	O
ATOM	3960	ND2	ASN	A	508	33.353	-0.622	32.729	1.00	31.05	N
ATOM	3961	C	ASN	A	508	30.945	-0.451	28.987	1.00	32.07	C
ATOM	3962	O	ASN	A	508	30.466	0.670	28.770	1.00	32.12	O
ATOM	3963	N	ASP	A	509	30.770	-1.515	28.204	1.00	32.85	N
ATOM	3964	CA	ASP	A	509	30.322	-1.472	26.796	1.00	33.78	C
ATOM	3965	CB	ASP	A	509	28.988	-0.734	26.585	1.00	35.51	C
ATOM	3966	CG	ASP	A	509	27.822	-1.707	26.333	1.00	39.61	C
ATOM	3967	OD1	ASP	A	509	28.108	-2.902	26.004	1.00	42.30	O
ATOM	3968	OD2	ASP	A	509	26.610	-1.353	26.447	1.00	43.47	O
ATOM	3969	C	ASP	A	509	31.385	-0.870	25.947	1.00	31.99	C
ATOM	3970	O	ASP	A	509	32.531	-0.921	26.285	1.00	32.56	O
ATOM	3971	N	TYR	A	510	31.029	-0.252	24.860	1.00	30.10	N
ATOM	3972	CA	TYR	A	510	32.083	0.203	23.984	1.00	29.03	C
ATOM	3973	CB	TYR	A	510	33.274	0.772	24.778	1.00	28.83	C

272/396

Figure 3A-72

ATOM	3974	CG	TYR	A	510	32.908	2.058	25.487	1.00	29.17	C
ATOM	3975	CD1	TYR	A	510	33.030	3.278	24.848	1.00	30.55	C
ATOM	3976	CE1	TYR	A	510	32.657	4.443	25.458	1.00	30.86	C
ATOM	3977	CZ	TYR	A	510	32.163	4.415	26.745	1.00	30.83	C
ATOM	3978	OH	TYR	A	510	31.791	5.611	27.367	1.00	34.61	O
ATOM	3979	CE2	TYR	A	510	32.036	3.220	27.397	1.00	29.34	C
ATOM	3980	CD2	TYR	A	510	32.391	2.052	26.762	1.00	28.92	C
ATOM	3981	C	TYR	A	510	32.494	-0.908	23.026	1.00	28.21	C
ATOM	3982	O	TYR	A	510	32.468	-2.101	23.361	1.00	27.32	O
ATOM	3983	N	SER	A	511	32.762	-0.474	21.801	1.00	27.62	N
ATOM	3984	CA	SER	A	511	33.336	-1.286	20.764	1.00	27.34	C
ATOM	3985	CB	SER	A	511	32.933	-0.702	19.410	1.00	27.55	C
ATOM	3986	OG	SER	A	511	33.413	0.651	19.271	1.00	26.66	O
ATOM	3987	C	SER	A	511	34.853	-1.092	20.924	1.00	27.45	C
ATOM	3988	O	SER	A	511	35.312	0.031	21.258	1.00	27.44	O
ATOM	3989	N	PHE	A	512	35.627	-2.148	20.672	1.00	26.24	N
ATOM	3990	CA	PHE	A	512	37.064	-1.985	20.614	1.00	25.63	C
ATOM	3991	CB	PHE	A	512	37.753	-3.201	21.244	1.00	26.08	C
ATOM	3992	CG	PHE	A	512	38.943	-2.856	22.099	1.00	24.71	C
ATOM	3993	CD1	PHE	A	512	40.198	-3.250	21.724	1.00	24.26	C
ATOM	3994	CE1	PHE	A	512	41.269	-2.933	22.499	1.00	26.07	C
ATOM	3995	CZ	PHE	A	512	41.076	-2.223	23.665	1.00	25.48	C
ATOM	3996	CE2	PHE	A	512	39.822	-1.829	24.040	1.00	22.11	C
ATOM	3997	CD2	PHE	A	512	38.783	-2.138	23.271	1.00	22.76	C
ATOM	3998	C	PHE	A	512	37.635	-1.654	19.212	1.00	25.27	C
ATOM	3999	O	PHE	A	512	38.457	-0.750	19.070	1.00	24.84	O
ATOM	4000	N	ILE	A	513	37.188	-2.380	18.190	1.00	24.73	N
ATOM	4001	CA	ILE	A	513	37.708	-2.241	16.818	1.00	24.43	C
ATOM	4002	CB	ILE	A	513	36.881	-3.146	15.802	1.00	24.16	C
ATOM	4003	CG1	ILE	A	513	37.748	-4.193	15.099	1.00	25.41	C
ATOM	4004	CD1	ILE	A	513	39.187	-4.402	15.659	1.00	26.52	C
ATOM	4005	CG2	ILE	A	513	36.215	-2.355	14.724	1.00	24.18	C
ATOM	4006	C	ILE	A	513	37.957	-0.802	16.301	1.00	24.12	C
ATOM	4007	O	ILE	A	513	38.655	-0.636	15.319	1.00	23.63	O
ATOM	4008	N	ARG	A	514	37.447	0.240	16.956	1.00	24.51	N
ATOM	4009	CA	ARG	A	514	37.848	1.596	16.519	1.00	25.83	C
ATOM	4010	CB	ARG	A	514	37.181	2.758	17.289	1.00	25.45	C
ATOM	4011	CG	ARG	A	514	36.138	2.344	18.307	1.00	28.05	C
ATOM	4012	CD	ARG	A	514	36.571	2.477	19.750	1.00	31.99	C
ATOM	4013	NE	ARG	A	514	35.925	3.606	20.409	1.00	33.72	N
ATOM	4014	CZ	ARG	A	514	34.731	3.544	20.996	1.00	36.46	C
ATOM	4015	NH1	ARG	A	514	34.031	2.381	21.012	1.00	34.26	N
ATOM	4016	NH2	ARG	A	514	34.236	4.663	21.562	1.00	37.14	N
ATOM	4017	C	ARG	A	514	39.350	1.650	16.701	1.00	26.20	C
ATOM	4018	O	ARG	A	514	40.125	1.978	15.771	1.00	25.94	O
ATOM	4019	N	TYR	A	515	39.712	1.253	17.925	1.00	26.54	N
ATOM	4020	CA	TYR	A	515	41.058	1.169	18.440	1.00	26.10	C
ATOM	4021	CB	TYR	A	515	41.038	0.324	19.681	1.00	24.76	C
ATOM	4022	CG	TYR	A	515	40.352	1.020	20.816	1.00	22.06	C
ATOM	4023	CD1	TYR	A	515	40.360	2.422	20.931	1.00	17.68	C
ATOM	4024	CE1	TYR	A	515	39.734	3.054	21.996	1.00	16.49	C
ATOM	4025	CZ	TYR	A	515	39.095	2.276	22.952	1.00	17.18	C
ATOM	4026	OH	TYR	A	515	38.443	2.821	24.044	1.00	16.57	O
ATOM	4027	CE2	TYR	A	515	39.088	0.899	22.846	1.00	17.28	C
ATOM	4028	CD2	TYR	A	515	39.707	0.285	21.794	1.00	19.62	C
ATOM	4029	C	TYR	A	515	42.004	0.600	17.427	1.00	27.32	C

273/396

Figure 3A-73

ATOM	4030	O	TYR	A	515	43.022	1.208	17.169	1.00	28.45	O
ATOM	4031	N	TYR	A	516	41.655	-0.529	16.827	1.00	28.05	N
ATOM	4032	CA	TYR	A	516	42.386	-1.056	15.694	1.00	28.99	C
ATOM	4033	CB	TYR	A	516	41.727	-2.324	15.237	1.00	28.94	C
ATOM	4034	CG	TYR	A	516	42.369	-2.959	14.041	1.00	29.88	C
ATOM	4035	CD1	TYR	A	516	42.976	-4.204	14.166	1.00	31.51	C
ATOM	4036	CE1	TYR	A	516	43.547	-4.823	13.092	1.00	32.64	C
ATOM	4037	CZ	TYR	A	516	43.533	-4.190	11.863	1.00	33.02	C
ATOM	4038	OH	TYR	A	516	44.110	-4.859	10.821	1.00	34.57	O
ATOM	4039	CE2	TYR	A	516	42.944	-2.932	11.695	1.00	31.27	C
ATOM	4040	CD2	TYR	A	516	42.349	-2.340	12.778	1.00	29.77	C
ATOM	4041	C	TYR	A	516	42.399	-0.107	14.495	1.00	30.03	C
ATOM	4042	O	TYR	A	516	43.489	0.241	13.983	1.00	30.97	O
ATOM	4043	N	THR	A	517	41.210	0.286	14.012	1.00	30.17	N
ATOM	4044	CA	THR	A	517	41.140	1.020	12.748	1.00	29.69	C
ATOM	4045	CB	THR	A	517	39.725	1.148	12.220	1.00	29.45	C
ATOM	4046	OG1	THR	A	517	38.866	1.544	13.287	1.00	27.93	O
ATOM	4047	CG2	THR	A	517	39.195	-0.222	11.749	1.00	29.11	C
ATOM	4048	C	THR	A	517	41.777	2.367	12.966	1.00	30.22	C
ATOM	4049	O	THR	A	517	42.588	2.794	12.137	1.00	30.38	O
ATOM	4050	N	ARG	A	518	41.473	3.009	14.101	1.00	30.58	N
ATOM	4051	CA	ARG	A	518	42.219	4.206	14.488	1.00	31.06	C
ATOM	4052	CB	ARG	A	518	42.213	4.472	15.982	1.00	30.75	C
ATOM	4053	CG	ARG	A	518	43.034	5.732	16.317	1.00	30.68	C
ATOM	4054	CD	ARG	A	518	44.383	5.529	17.053	1.00	31.49	C
ATOM	4055	NE	ARG	A	518	44.342	5.952	18.463	1.00	30.80	N
ATOM	4056	CZ	ARG	A	518	44.133	5.116	19.501	1.00	31.07	C
ATOM	4057	NH1	ARG	A	518	44.087	5.588	20.747	1.00	31.24	N
ATOM	4058	NH2	ARG	A	518	43.967	3.805	19.299	1.00	28.89	N
ATOM	4059	C	ARG	A	518	43.656	4.011	14.111	1.00	31.87	C
ATOM	4060	O	ARG	A	518	44.237	4.885	13.491	1.00	32.06	O
ATOM	4061	N	THR	A	519	44.214	2.850	14.487	1.00	32.97	N
ATOM	4062	CA	THR	A	519	45.658	2.585	14.412	1.00	33.86	C
ATOM	4063	CB	THR	A	519	46.065	1.200	15.011	1.00	33.79	C
ATOM	4064	OG1	THR	A	519	46.068	1.297	16.438	1.00	34.53	O
ATOM	4065	CG2	THR	A	519	47.527	0.876	14.730	1.00	33.14	C
ATOM	4066	C	THR	A	519	46.221	2.787	13.020	1.00	34.63	C
ATOM	4067	O	THR	A	519	47.382	3.254	12.927	1.00	34.91	O
ATOM	4068	N	LEU	A	520	45.421	2.466	11.975	1.00	34.62	N
ATOM	4069	CA	LEU	A	520	45.728	2.892	10.589	1.00	34.81	C
ATOM	4070	CB	LEU	A	520	45.014	2.083	9.551	1.00	34.00	C
ATOM	4071	CG	LEU	A	520	45.471	0.655	9.625	1.00	34.88	C
ATOM	4072	CD1	LEU	A	520	45.099	0.045	10.983	1.00	35.65	C
ATOM	4073	CD2	LEU	A	520	44.857	-0.147	8.474	1.00	35.93	C
ATOM	4074	C	LEU	A	520	45.414	4.352	10.351	1.00	35.51	C
ATOM	4075	O	LEU	A	520	46.287	5.207	10.520	1.00	35.27	O
ATOM	4076	N	TYR	A	521	44.178	4.662	9.975	1.00	36.41	N
ATOM	4077	CA	TYR	A	521	43.870	6.037	9.599	1.00	37.30	C
ATOM	4078	CB	TYR	A	521	42.525	6.484	10.141	1.00	37.38	C
ATOM	4079	CG	TYR	A	521	41.336	5.595	9.932	1.00	37.12	C
ATOM	4080	CD1	TYR	A	521	40.715	5.471	8.697	1.00	37.35	C
ATOM	4081	CE1	TYR	A	521	39.572	4.678	8.550	1.00	38.46	C
ATOM	4082	CZ	TYR	A	521	39.042	4.042	9.673	1.00	40.12	C
ATOM	4083	OH	TYR	A	521	37.918	3.227	9.653	1.00	40.84	O
ATOM	4084	CE2	TYR	A	521	39.642	4.204	10.893	1.00	40.23	C
ATOM	4085	CD2	TYR	A	521	40.765	4.972	11.013	1.00	38.49	C

274/396

Figure 3A-74

ATOM	4086	C	TYR	A	521	44.936	7.032	10.101	1.00	37.70	C
ATOM	4087	O	TYR	A	521	45.228	8.027	9.447	1.00	37.70	O
ATOM	4088	N	GLN	A	522	45.497	6.739	11.269	1.00	38.51	N
ATOM	4089	CA	GLN	A	522	46.552	7.529	11.903	1.00	39.82	C
ATOM	4090	CB	GLN	A	522	47.242	6.671	12.969	1.00	40.42	C
ATOM	4091	CG	GLN	A	522	47.824	7.450	14.157	1.00	43.64	C
ATOM	4092	CD	GLN	A	522	48.249	6.522	15.291	1.00	48.32	C
ATOM	4093	OE1	GLN	A	522	47.809	5.351	15.353	1.00	50.10	O
ATOM	4094	NE2	GLN	A	522	49.093	7.031	16.194	1.00	48.67	N
ATOM	4095	C	GLN	A	522	47.601	7.979	10.912	1.00	39.43	C
ATOM	4096	O	GLN	A	522	47.820	9.174	10.658	1.00	39.25	O
ATOM	4097	N	PHE	A	523	48.265	6.994	10.355	1.00	39.33	N
ATOM	4098	CA	PHE	A	523	49.291	7.275	9.390	1.00	39.93	C
ATOM	4099	CB	PHE	A	523	50.217	6.066	9.332	1.00	39.69	C
ATOM	4100	CG	PHE	A	523	50.697	5.694	10.687	1.00	39.34	C
ATOM	4101	CD1	PHE	A	523	51.715	6.417	11.285	1.00	38.66	C
ATOM	4102	CE1	PHE	A	523	52.119	6.115	12.571	1.00	40.54	C
ATOM	4103	CZ	PHE	A	523	51.473	5.099	13.309	1.00	40.34	C
ATOM	4104	CE2	PHE	A	523	50.438	4.406	12.735	1.00	40.91	C
ATOM	4105	CD2	PHE	A	523	50.041	4.720	11.428	1.00	40.55	C
ATOM	4106	C	PHE	A	523	48.688	7.784	8.059	1.00	40.55	C
ATOM	4107	O	PHE	A	523	49.188	8.754	7.473	1.00	40.50	O
ATOM	4108	N	GLN	A	524	47.562	7.179	7.657	1.00	40.92	N
ATOM	4109	CA	GLN	A	524	46.830	7.560	6.470	1.00	40.41	C
ATOM	4110	CB	GLN	A	524	45.519	6.854	6.413	1.00	39.70	C
ATOM	4111	CG	GLN	A	524	45.339	6.228	5.087	1.00	39.00	C
ATOM	4112	CD	GLN	A	524	44.589	4.929	5.178	1.00	37.16	C
ATOM	4113	OE1	GLN	A	524	44.380	4.288	4.158	1.00	35.70	O
ATOM	4114	NE2	GLN	A	524	44.186	4.533	6.389	1.00	34.62	N
ATOM	4115	C	GLN	A	524	46.586	9.016	6.470	1.00	41.25	C
ATOM	4116	O	GLN	A	524	46.857	9.653	5.483	1.00	41.51	O
ATOM	4117	N	PHE	A	525	46.103	9.556	7.578	1.00	42.68	N
ATOM	4118	CA	PHE	A	525	45.961	11.006	7.701	1.00	44.82	C
ATOM	4119	CB	PHE	A	525	45.078	11.397	8.885	1.00	44.51	C
ATOM	4120	CG	PHE	A	525	43.634	11.032	8.734	1.00	43.66	C
ATOM	4121	CD1	PHE	A	525	43.234	9.960	7.943	1.00	43.38	C
ATOM	4122	CE1	PHE	A	525	41.910	9.608	7.837	1.00	41.71	C
ATOM	4123	CZ	PHE	A	525	40.978	10.312	8.528	1.00	41.42	C
ATOM	4124	CE2	PHE	A	525	41.360	11.386	9.317	1.00	42.06	C
ATOM	4125	CD2	PHE	A	525	42.674	11.742	9.415	1.00	42.06	C
ATOM	4126	C	PHE	A	525	47.313	11.717	7.840	1.00	46.64	C
ATOM	4127	O	PHE	A	525	47.443	12.936	7.554	1.00	46.90	O
ATOM	4128	N	GLN	A	526	48.316	10.967	8.285	1.00	48.53	N
ATOM	4129	CA	GLN	A	526	49.632	11.551	8.442	1.00	50.35	C
ATOM	4130	CB	GLN	A	526	50.417	10.858	9.553	1.00	50.50	C
ATOM	4131	CG	GLN	A	526	51.580	11.679	10.087	1.00	51.93	C
ATOM	4132	CD	GLN	A	526	51.158	13.017	10.621	1.00	53.17	C
ATOM	4133	OE1	GLN	A	526	51.863	13.602	11.438	1.00	55.37	O
ATOM	4134	NE2	GLN	A	526	50.013	13.514	10.166	1.00	53.08	N
ATOM	4135	C	GLN	A	526	50.426	11.729	7.124	1.00	51.15	C
ATOM	4136	O	GLN	A	526	50.919	12.822	6.880	1.00	51.39	O
ATOM	4137	N	GLU	A	527	50.521	10.715	6.260	1.00	52.23	N
ATOM	4138	CA	GLU	A	527	51.192	10.918	4.958	1.00	53.86	C
ATOM	4139	CB	GLU	A	527	51.139	9.669	4.033	1.00	54.42	C
ATOM	4140	CG	GLU	A	527	52.423	9.365	3.217	1.00	58.89	C
ATOM	4141	CD	GLU	A	527	52.442	7.976	2.469	1.00	65.89	C

275/396

Figure 3A-75

ATOM	4142	OE1	GLU	A	527	51.647	7.757	1.473	1.00	67.03	O
ATOM	4143	OE2	GLU	A	527	53.289	7.086	2.846	1.00	67.18	O
ATOM	4144	C	GLU	A	527	50.564	12.139	4.290	1.00	53.75	C
ATOM	4145	O	GLU	A	527	51.220	12.853	3.538	1.00	54.21	O
ATOM	4146	N	ALA	A	528	49.306	12.395	4.624	1.00	53.60	N
ATOM	4147	CA	ALA	A	528	48.549	13.475	4.040	1.00	53.55	C
ATOM	4148	CB	ALA	A	528	47.092	13.177	4.136	1.00	53.91	C
ATOM	4149	C	ALA	A	528	48.847	14.825	4.653	1.00	53.72	C
ATOM	4150	O	ALA	A	528	49.245	15.730	3.948	1.00	53.52	O
ATOM	4151	N	LEU	A	529	48.654	14.986	5.950	1.00	54.23	N
ATOM	4152	CA	LEU	A	529	48.907	16.290	6.540	1.00	55.66	C
ATOM	4153	CB	LEU	A	529	48.389	16.303	7.947	1.00	54.86	C
ATOM	4154	CG	LEU	A	529	46.954	15.845	7.950	1.00	53.79	C
ATOM	4155	CD1	LEU	A	529	46.873	14.711	8.889	1.00	53.32	C
ATOM	4156	CD2	LEU	A	529	46.037	16.967	8.398	1.00	53.63	C
ATOM	4157	C	LEU	A	529	50.379	16.793	6.477	1.00	57.67	C
ATOM	4158	O	LEU	A	529	50.644	17.999	6.489	1.00	57.75	O
ATOM	4159	N	CYS	A	530	51.326	15.861	6.402	1.00	59.91	N
ATOM	4160	CA	CYS	A	530	52.746	16.166	6.205	1.00	62.08	C
ATOM	4161	CB	CYS	A	530	53.563	14.882	6.290	1.00	62.53	C
ATOM	4162	SG	CYS	A	530	53.624	14.341	8.011	1.00	67.44	S
ATOM	4163	C	CYS	A	530	53.016	16.872	4.888	1.00	62.58	C
ATOM	4164	O	CYS	A	530	53.411	18.030	4.884	1.00	62.77	O
ATOM	4165	N	GLN	A	531	52.810	16.167	3.777	1.00	63.43	N
ATOM	4166	CA	GLN	A	531	52.748	16.786	2.452	1.00	64.21	C
ATOM	4167	CB	GLN	A	531	51.931	15.900	1.495	1.00	64.55	C
ATOM	4168	CG	GLN	A	531	52.759	15.164	0.419	1.00	66.58	C
ATOM	4169	CD	GLN	A	531	52.172	13.791	-0.017	1.00	68.80	C
ATOM	4170	OE1	GLN	A	531	52.171	13.442	-1.215	1.00	68.10	O
ATOM	4171	NE2	GLN	A	531	51.695	13.012	0.959	1.00	70.12	N
ATOM	4172	C	GLN	A	531	52.098	18.166	2.544	1.00	64.15	C
ATOM	4173	O	GLN	A	531	52.343	19.038	1.705	1.00	63.89	O
ATOM	4174	N	ALA	A	532	51.275	18.334	3.582	1.00	64.52	N
ATOM	4175	CA	ALA	A	532	50.461	19.524	3.799	1.00	65.00	C
ATOM	4176	CB	ALA	A	532	49.036	19.124	4.079	1.00	64.80	C
ATOM	4177	C	ALA	A	532	50.993	20.375	4.936	1.00	65.44	C
ATOM	4178	O	ALA	A	532	50.261	21.171	5.513	1.00	65.44	O
ATOM	4179	N	ALA	A	533	52.258	20.164	5.281	1.00	66.11	N
ATOM	4180	CA	ALA	A	533	53.018	21.068	6.145	1.00	66.64	C
ATOM	4181	CB	ALA	A	533	53.462	20.351	7.399	1.00	66.27	C
ATOM	4182	C	ALA	A	533	54.235	21.511	5.364	1.00	67.08	C
ATOM	4183	O	ALA	A	533	54.995	22.366	5.813	1.00	67.20	O
ATOM	4184	N	LYS	A	534	54.362	20.933	4.166	1.00	67.79	N
ATOM	4185	CA	LYS	A	534	55.643	20.660	3.476	1.00	68.47	C
ATOM	4186	CB	LYS	A	534	56.353	21.937	3.001	1.00	68.32	C
ATOM	4187	CG	LYS	A	534	57.626	21.655	2.198	1.00	69.24	C
ATOM	4188	CD	LYS	A	534	57.407	21.757	0.677	1.00	71.33	C
ATOM	4189	CE	LYS	A	534	58.314	20.786	-0.112	1.00	71.57	C
ATOM	4190	NZ	LYS	A	534	57.816	19.360	-0.060	1.00	71.34	N
ATOM	4191	C	LYS	A	534	56.584	19.716	4.277	1.00	68.58	C
ATOM	4192	O	LYS	A	534	56.945	20.027	5.410	1.00	69.20	O
ATOM	4193	N	HIS	A	535	56.952	18.566	3.709	1.00	68.48	N
ATOM	4194	CA	HIS	A	535	57.875	17.679	4.393	1.00	68.90	C
ATOM	4195	CB	HIS	A	535	57.138	16.704	5.302	1.00	69.01	C
ATOM	4196	CG	HIS	A	535	58.058	15.891	6.160	1.00	71.03	C
ATOM	4197	ND1	HIS	A	535	59.140	16.440	6.820	1.00	72.57	N

276/396

Figure 3A-76

ATOM	4198	CE1	HIS	A	535	59.780	15.494	7.483	1.00	72.35	C
ATOM	4199	NE2	HIS	A	535	59.156	14.348	7.276	1.00	72.71	N
ATOM	4200	CD2	HIS	A	535	58.075	14.568	6.450	1.00	72.33	C
ATOM	4201	C	HIS	A	535	58.916	16.955	3.530	1.00	69.11	C
ATOM	4202	O	HIS	A	535	58.587	16.211	2.606	1.00	69.12	O
ATOM	4203	N	GLU	A	536	60.179	17.194	3.878	1.00	69.83	N
ATOM	4204	CA	GLU	A	536	61.381	16.635	3.215	1.00	70.70	C
ATOM	4205	CB	GLU	A	536	62.286	17.785	2.676	1.00	70.96	C
ATOM	4206	CG	GLU	A	536	62.491	17.902	1.152	1.00	71.75	C
ATOM	4207	CD	GLU	A	536	61.238	18.290	0.336	1.00	73.34	C
ATOM	4208	OE1	GLU	A	536	61.067	19.509	0.026	1.00	73.14	O
ATOM	4209	OE2	GLU	A	536	60.433	17.380	-0.028	1.00	73.05	O
ATOM	4210	C	GLU	A	536	62.155	15.704	4.205	1.00	70.75	C
ATOM	4211	O	GLU	A	536	63.386	15.793	4.392	1.00	70.61	O
ATOM	4212	N	GLY	A	537	61.390	14.841	4.864	1.00	70.69	N
ATOM	4213	CA	GLY	A	537	61.906	13.849	5.782	1.00	70.48	C
ATOM	4214	C	GLY	A	537	60.817	12.808	5.802	1.00	70.41	C
ATOM	4215	O	GLY	A	537	59.771	13.001	5.176	1.00	70.62	O
ATOM	4216	N	PRO	A	538	61.037	11.704	6.491	1.00	70.40	N
ATOM	4217	CA	PRO	A	538	60.017	10.651	6.599	1.00	70.61	C
ATOM	4218	CB	PRO	A	538	60.800	9.473	7.178	1.00	70.78	C
ATOM	4219	CG	PRO	A	538	62.240	9.871	6.995	1.00	70.87	C
ATOM	4220	CD	PRO	A	538	62.272	11.355	7.200	1.00	70.31	C
ATOM	4221	C	PRO	A	538	58.886	11.068	7.541	1.00	70.56	C
ATOM	4222	O	PRO	A	538	59.030	12.085	8.229	1.00	70.75	O
ATOM	4223	N	LEU	A	539	57.785	10.322	7.584	1.00	70.36	N
ATOM	4224	CA	LEU	A	539	56.653	10.783	8.394	1.00	70.37	C
ATOM	4225	CB	LEU	A	539	55.306	10.181	7.963	1.00	70.18	C
ATOM	4226	CG	LEU	A	539	54.923	8.728	8.148	1.00	69.26	C
ATOM	4227	CD1	LEU	A	539	53.489	8.694	8.596	1.00	67.23	C
ATOM	4228	CD2	LEU	A	539	55.121	7.979	6.829	1.00	69.99	C
ATOM	4229	C	LEU	A	539	56.894	10.606	9.869	1.00	70.55	C
ATOM	4230	O	LEU	A	539	56.430	11.403	10.686	1.00	70.37	O
ATOM	4231	N	HIS	A	540	57.652	9.567	10.195	1.00	70.97	N
ATOM	4232	CA	HIS	A	540	57.988	9.290	11.576	1.00	71.46	C
ATOM	4233	CB	HIS	A	540	58.697	7.930	11.707	1.00	71.80	C
ATOM	4234	CG	HIS	A	540	60.154	7.942	11.356	1.00	73.40	C
ATOM	4235	ND1	HIS	A	540	60.788	6.847	10.805	1.00	74.71	N
ATOM	4236	CE1	HIS	A	540	62.070	7.122	10.632	1.00	75.86	C
ATOM	4237	NE2	HIS	A	540	62.290	8.356	11.053	1.00	76.52	N
ATOM	4238	CD2	HIS	A	540	61.112	8.884	11.524	1.00	74.70	C
ATOM	4239	C	HIS	A	540	58.724	10.443	12.268	1.00	71.31	C
ATOM	4240	O	HIS	A	540	58.595	10.615	13.483	1.00	71.64	O
ATOM	4241	N	LYS	A	541	59.452	11.249	11.491	1.00	70.88	N
ATOM	4242	CA	LYS	A	541	60.087	12.461	11.999	1.00	70.39	C
ATOM	4243	CB	LYS	A	541	61.430	12.739	11.300	1.00	70.47	C
ATOM	4244	CG	LYS	A	541	62.589	11.813	11.653	1.00	70.65	C
ATOM	4245	CD	LYS	A	541	63.209	12.167	12.986	1.00	70.91	C
ATOM	4246	CE	LYS	A	541	64.658	12.566	12.830	1.00	71.38	C
ATOM	4247	NZ	LYS	A	541	65.305	12.762	14.174	1.00	71.76	N
ATOM	4248	C	LYS	A	541	59.160	13.636	11.773	1.00	70.10	C
ATOM	4249	O	LYS	A	541	59.473	14.757	12.160	1.00	70.08	O
ATOM	4250	N	CYS	A	542	58.018	13.391	11.144	1.00	69.89	N
ATOM	4251	CA	CYS	A	542	57.140	14.493	10.773	1.00	70.39	C
ATOM	4252	CB	CYS	A	542	56.085	14.039	9.765	1.00	70.53	C
ATOM	4253	SG	CYS	A	542	55.115	15.367	8.963	1.00	70.87	S

277/396

Figure 3A-77

ATOM	4254	C	CYS	A	542	56.464	15.257	11.926	1.00	70.57	C
ATOM	4255	O	CYS	A	542	55.714	14.684	12.755	1.00	70.70	O
ATOM	4256	N	ASP	A	543	56.736	16.563	11.923	1.00	70.33	N
ATOM	4257	CA	ASP	A	543	56.087	17.585	12.748	1.00	70.08	C
ATOM	4258	CB	ASP	A	543	56.927	18.840	12.648	1.00	70.72	C
ATOM	4259	CG	ASP	A	543	57.111	19.291	11.173	1.00	72.69	C
ATOM	4260	OD1	ASP	A	543	56.613	20.411	10.836	1.00	73.19	O
ATOM	4261	OD2	ASP	A	543	57.712	18.572	10.296	1.00	73.57	O
ATOM	4262	C	ASP	A	543	54.709	17.975	12.214	1.00	69.17	C
ATOM	4263	O	ASP	A	543	54.099	17.271	11.409	1.00	68.96	O
ATOM	4264	N	ILE	A	544	54.243	19.138	12.656	1.00	68.26	N
ATOM	4265	CA	ILE	A	544	53.010	19.751	12.159	1.00	67.32	C
ATOM	4266	CB	ILE	A	544	51.781	18.781	12.225	1.00	67.35	C
ATOM	4267	CG1	ILE	A	544	50.608	19.345	11.434	1.00	66.71	C
ATOM	4268	CD1	ILE	A	544	49.397	19.655	12.290	1.00	66.05	C
ATOM	4269	CG2	ILE	A	544	51.346	18.480	13.683	1.00	67.59	C
ATOM	4270	C	ILE	A	544	52.760	21.021	12.953	1.00	66.75	C
ATOM	4271	O	ILE	A	544	52.277	22.010	12.404	1.00	66.29	O
ATOM	4272	N	SER	A	545	53.117	20.990	14.240	1.00	66.26	N
ATOM	4273	CA	SER	A	545	52.942	22.151	15.106	1.00	66.01	C
ATOM	4274	CB	SER	A	545	53.880	22.118	16.349	1.00	66.26	C
ATOM	4275	OG	SER	A	545	53.464	22.986	17.418	1.00	65.17	O
ATOM	4276	C	SER	A	545	53.154	23.398	14.246	1.00	65.71	C
ATOM	4277	O	SER	A	545	54.214	23.571	13.618	1.00	65.84	O
ATOM	4278	N	ASN	A	546	52.097	24.213	14.183	1.00	65.12	N
ATOM	4279	CA	ASN	A	546	52.092	25.549	13.576	1.00	64.24	C
ATOM	4280	CB	ASN	A	546	53.494	26.197	13.609	1.00	64.34	C
ATOM	4281	CG	ASN	A	546	53.994	26.451	15.032	1.00	62.97	C
ATOM	4282	OD1	ASN	A	546	54.470	25.543	15.729	1.00	59.76	O
ATOM	4283	ND2	ASN	A	546	53.894	27.698	15.457	1.00	63.16	N
ATOM	4284	C	ASN	A	546	51.427	25.647	12.184	1.00	63.59	C
ATOM	4285	O	ASN	A	546	50.791	26.665	11.864	1.00	63.48	O
ATOM	4286	N	SER	A	547	51.559	24.595	11.376	1.00	62.48	N
ATOM	4287	CA	SER	A	547	50.982	24.592	10.027	1.00	61.52	C
ATOM	4288	CB	SER	A	547	51.526	23.415	9.200	1.00	61.50	C
ATOM	4289	OG	SER	A	547	50.632	23.060	8.156	1.00	60.31	O
ATOM	4290	C	SER	A	547	49.453	24.552	10.036	1.00	60.89	C
ATOM	4291	O	SER	A	547	48.877	23.526	10.446	1.00	60.55	O
ATOM	4292	N	THR	A	548	48.810	25.655	9.590	1.00	60.00	N
ATOM	4293	CA	THR	A	548	47.335	25.688	9.381	1.00	58.71	C
ATOM	4294	CB	THR	A	548	46.722	27.086	9.494	1.00	57.99	C
ATOM	4295	OG1	THR	A	548	47.452	27.987	8.660	1.00	57.38	O
ATOM	4296	CG2	THR	A	548	46.866	27.632	10.882	1.00	56.39	C
ATOM	4297	C	THR	A	548	46.953	25.069	8.035	1.00	58.75	C
ATOM	4298	O	THR	A	548	45.885	24.448	7.909	1.00	58.39	O
ATOM	4299	N	GLU	A	549	47.822	25.237	7.037	1.00	58.27	N
ATOM	4300	CA	GLU	A	549	47.786	24.377	5.864	1.00	58.44	C
ATOM	4301	CB	GLU	A	549	49.179	24.289	5.270	1.00	58.82	C
ATOM	4302	CG	GLU	A	549	50.036	25.474	5.604	1.00	60.81	C
ATOM	4303	CD	GLU	A	549	49.706	26.629	4.695	1.00	64.26	C
ATOM	4304	OE1	GLU	A	549	50.101	26.518	3.502	1.00	65.41	O
ATOM	4305	OE2	GLU	A	549	49.037	27.607	5.162	1.00	64.32	O
ATOM	4306	C	GLU	A	549	47.382	22.972	6.308	1.00	57.98	C
ATOM	4307	O	GLU	A	549	46.596	22.270	5.640	1.00	58.10	O
ATOM	4308	N	ALA	A	550	47.949	22.589	7.450	1.00	57.20	N
ATOM	4309	CA	ALA	A	550	47.734	21.302	8.076	1.00	56.51	C

278/396

Figure 3A-78

ATOM	4310	CB	ALA	A	550	48.906	20.983	8.969	1.00	56.89	C
ATOM	4311	C	ALA	A	550	46.456	21.269	8.884	1.00	55.70	C
ATOM	4312	O	ALA	A	550	45.686	20.314	8.801	1.00	55.52	O
ATOM	4313	N	GLY	A	551	46.252	22.299	9.690	1.00	54.93	N
ATOM	4314	CA	GLY	A	551	45.043	22.400	10.471	1.00	54.67	C
ATOM	4315	C	GLY	A	551	43.848	22.429	9.550	1.00	54.41	C
ATOM	4316	O	GLY	A	551	42.890	21.677	9.747	1.00	53.95	O
ATOM	4317	N	GLN	A	552	43.939	23.276	8.522	1.00	54.31	N
ATOM	4318	CA	GLN	A	552	42.869	23.438	7.540	1.00	54.43	C
ATOM	4319	CB	GLN	A	552	43.291	24.345	6.382	1.00	54.09	C
ATOM	4320	CG	GLN	A	552	42.129	25.200	5.827	1.00	56.22	C
ATOM	4321	CD	GLN	A	552	41.041	25.600	6.874	1.00	58.09	C
ATOM	4322	OE1	GLN	A	552	41.049	26.737	7.404	1.00	58.81	O
ATOM	4323	NE2	GLN	A	552	40.106	24.676	7.153	1.00	57.71	N
ATOM	4324	C	GLN	A	552	42.279	22.116	7.044	1.00	54.12	C
ATOM	4325	O	GLN	A	552	41.127	21.806	7.349	1.00	53.99	O
ATOM	4326	N	LYS	A	553	43.069	21.335	6.312	1.00	54.07	N
ATOM	4327	CA	LYS	A	553	42.649	19.989	5.943	1.00	54.25	C
ATOM	4328	CB	LYS	A	553	43.836	19.120	5.464	1.00	53.90	C
ATOM	4329	CG	LYS	A	553	43.937	18.971	3.922	1.00	53.53	C
ATOM	4330	CD	LYS	A	553	43.948	17.496	3.413	1.00	53.44	C
ATOM	4331	CE	LYS	A	553	43.932	17.361	1.852	1.00	54.57	C
ATOM	4332	NZ	LYS	A	553	42.845	16.498	1.216	1.00	52.03	N
ATOM	4333	C	LYS	A	553	41.851	19.342	7.105	1.00	54.51	C
ATOM	4334	O	LYS	A	553	40.654	19.043	6.956	1.00	55.16	O
ATOM	4335	N	LEU	A	554	42.476	19.165	8.266	1.00	54.26	N
ATOM	4336	CA	LEU	A	554	41.766	18.553	9.389	1.00	53.72	C
ATOM	4337	CB	LEU	A	554	42.576	18.657	10.693	1.00	53.67	C
ATOM	4338	CG	LEU	A	554	42.160	17.611	11.720	1.00	52.31	C
ATOM	4339	CD1	LEU	A	554	42.207	16.235	11.087	1.00	50.64	C
ATOM	4340	CD2	LEU	A	554	43.023	17.706	12.940	1.00	51.51	C
ATOM	4341	C	LEU	A	554	40.379	19.174	9.553	1.00	53.37	C
ATOM	4342	O	LEU	A	554	39.375	18.504	9.372	1.00	53.35	O
ATOM	4343	N	PHE	A	555	40.344	20.458	9.898	1.00	52.95	N
ATOM	4344	CA	PHE	A	555	39.101	21.214	10.038	1.00	52.51	C
ATOM	4345	CB	PHE	A	555	39.402	22.744	10.060	1.00	53.09	C
ATOM	4346	CG	PHE	A	555	38.446	23.604	10.910	1.00	52.83	C
ATOM	4347	CD1	PHE	A	555	37.074	23.303	11.026	1.00	52.26	C
ATOM	4348	CE1	PHE	A	555	36.210	24.129	11.778	1.00	53.65	C
ATOM	4349	CZ	PHE	A	555	36.719	25.305	12.414	1.00	54.50	C
ATOM	4350	CE2	PHE	A	555	38.097	25.624	12.287	1.00	53.77	C
ATOM	4351	CD2	PHE	A	555	38.937	24.774	11.526	1.00	52.90	C
ATOM	4352	C	PHE	A	555	38.212	20.828	8.852	1.00	51.66	C
ATOM	4353	O	PHE	A	555	37.289	20.016	9.021	1.00	51.58	O
ATOM	4354	N	ASN	A	556	38.511	21.378	7.666	1.00	50.19	N
ATOM	4355	CA	ASN	A	556	37.705	21.156	6.466	1.00	48.99	C
ATOM	4356	CB	ASN	A	556	38.478	21.511	5.180	1.00	48.99	C
ATOM	4357	CG	ASN	A	556	38.800	22.984	5.051	1.00	48.98	C
ATOM	4358	OD1	ASN	A	556	39.933	23.351	4.740	1.00	47.65	O
ATOM	4359	ND2	ASN	A	556	37.804	23.837	5.254	1.00	50.58	N
ATOM	4360	C	ASN	A	556	37.269	19.713	6.321	1.00	48.24	C
ATOM	4361	O	ASN	A	556	36.894	19.318	5.236	1.00	48.84	O
ATOM	4362	N	MET	A	557	37.332	18.924	7.389	1.00	47.12	N
ATOM	4363	CA	MET	A	557	37.140	17.473	7.305	1.00	46.18	C
ATOM	4364	CB	MET	A	557	38.502	16.804	6.994	1.00	46.71	C
ATOM	4365	CG	MET	A	557	39.178	16.026	8.130	1.00	48.50	C

279/396

Figure 3A-79

ATOM	4366	SD	MET	A	557	38.364	14.418	8.352	1.00	52.92	S
ATOM	4367	CE	MET	A	557	38.946	13.966	10.003	1.00	51.73	C
ATOM	4368	C	MET	A	557	36.493	16.959	8.593	1.00	44.77	C
ATOM	4369	O	MET	A	557	35.731	15.993	8.627	1.00	43.60	O
ATOM	4370	N	LEU	A	558	36.824	17.667	9.648	1.00	43.95	N
ATOM	4371	CA	LEU	A	558	36.366	17.375	10.952	1.00	43.70	C
ATOM	4372	CB	LEU	A	558	37.063	18.327	11.886	1.00	43.32	C
ATOM	4373	CG	LEU	A	558	38.219	17.727	12.649	1.00	43.58	C
ATOM	4374	CD1	LEU	A	558	38.664	16.401	12.059	1.00	43.13	C
ATOM	4375	CD2	LEU	A	558	39.337	18.732	12.626	1.00	45.35	C
ATOM	4376	C	LEU	A	558	34.902	17.677	10.987	1.00	44.04	C
ATOM	4377	O	LEU	A	558	34.055	16.778	11.154	1.00	44.16	O
ATOM	4378	N	ARG	A	559	34.631	18.974	10.840	1.00	44.15	N
ATOM	4379	CA	ARG	A	559	33.289	19.550	10.762	1.00	43.99	C
ATOM	4380	CB	ARG	A	559	33.375	21.072	10.529	1.00	44.22	C
ATOM	4381	CG	ARG	A	559	34.358	21.483	9.425	1.00	47.31	C
ATOM	4382	CD	ARG	A	559	33.946	21.026	7.982	1.00	55.45	C
ATOM	4383	NE	ARG	A	559	33.620	22.104	7.009	1.00	62.30	N
ATOM	4384	CZ	ARG	A	559	32.636	23.040	7.121	1.00	64.65	C
ATOM	4385	NH1	ARG	A	559	31.794	23.096	8.182	1.00	63.78	N
ATOM	4386	NH2	ARG	A	559	32.508	23.942	6.142	1.00	65.29	N
ATOM	4387	C	ARG	A	559	32.524	18.974	9.604	1.00	42.80	C
ATOM	4388	O	ARG	A	559	32.191	19.709	8.714	1.00	42.87	O
ATOM	4389	N	LEU	A	560	32.282	17.675	9.567	1.00	41.48	N
ATOM	4390	CA	LEU	A	560	31.352	17.169	8.594	1.00	40.43	C
ATOM	4391	CB	LEU	A	560	32.051	16.511	7.404	1.00	40.46	C
ATOM	4392	CG	LEU	A	560	32.591	17.322	6.193	1.00	42.20	C
ATOM	4393	CD1	LEU	A	560	31.617	18.309	5.467	1.00	44.55	C
ATOM	4394	CD2	LEU	A	560	33.896	18.026	6.492	1.00	42.79	C
ATOM	4395	C	LEU	A	560	30.409	16.232	9.289	1.00	39.89	C
ATOM	4396	O	LEU	A	560	29.496	15.744	8.658	1.00	40.26	O
ATOM	4397	N	GLY	A	561	30.616	16.006	10.592	1.00	39.30	N
ATOM	4398	CA	GLY	A	561	29.787	15.112	11.409	1.00	38.89	C
ATOM	4399	C	GLY	A	561	29.754	13.726	10.806	1.00	38.76	C
ATOM	4400	O	GLY	A	561	30.632	13.437	10.009	1.00	38.62	O
ATOM	4401	N	LYS	A	562	28.760	12.891	11.143	1.00	39.07	N
ATOM	4402	CA	LYS	A	562	28.483	11.612	10.403	1.00	39.41	C
ATOM	4403	CB	LYS	A	562	27.756	10.602	11.308	1.00	39.36	C
ATOM	4404	CG	LYS	A	562	27.991	9.139	10.930	1.00	40.75	C
ATOM	4405	CD	LYS	A	562	28.012	8.232	12.177	1.00	44.76	C
ATOM	4406	CE	LYS	A	562	28.563	6.787	11.907	1.00	44.92	C
ATOM	4407	NZ	LYS	A	562	28.102	5.779	12.956	1.00	44.11	N
ATOM	4408	C	LYS	A	562	27.720	11.704	9.047	1.00	39.14	C
ATOM	4409	O	LYS	A	562	26.855	10.872	8.766	1.00	38.90	O
ATOM	4410	N	SER	A	563	28.075	12.660	8.194	1.00	39.21	N
ATOM	4411	CA	SER	A	563	27.144	13.119	7.170	1.00	40.03	C
ATOM	4412	CB	SER	A	563	26.589	14.490	7.599	1.00	40.05	C
ATOM	4413	OG	SER	A	563	27.152	15.537	6.829	1.00	41.33	O
ATOM	4414	C	SER	A	563	27.736	13.181	5.766	1.00	40.38	C
ATOM	4415	O	SER	A	563	27.488	14.127	5.008	1.00	40.57	O
ATOM	4416	N	GLU	A	564	28.505	12.157	5.430	1.00	40.96	N
ATOM	4417	CA	GLU	A	564	29.354	12.103	4.246	1.00	41.81	C
ATOM	4418	CB	GLU	A	564	30.463	13.189	4.296	1.00	42.42	C
ATOM	4419	CG	GLU	A	564	30.258	14.544	3.591	1.00	43.32	C
ATOM	4420	CD	GLU	A	564	30.770	14.609	2.141	1.00	43.55	C
ATOM	4421	OE1	GLU	A	564	30.520	13.631	1.396	1.00	45.92	O

280/396

Figure 3A-80

ATOM	4422	OE2	GLU	A	564	31.356	15.647	1.722	1.00	39.43	O
ATOM	4423	C	GLU	A	564	30.035	10.793	4.576	1.00	42.38	C
ATOM	4424	O	GLU	A	564	30.820	10.774	5.531	1.00	42.55	O
ATOM	4425	N	PRO	A	565	29.734	9.689	3.885	1.00	42.78	N
ATOM	4426	CA	PRO	A	565	30.417	8.404	4.133	1.00	43.23	C
ATOM	4427	CB	PRO	A	565	30.060	7.591	2.884	1.00	43.18	C
ATOM	4428	CG	PRO	A	565	28.671	7.989	2.646	1.00	43.06	C
ATOM	4429	CD	PRO	A	565	28.672	9.512	2.886	1.00	43.16	C
ATOM	4430	C	PRO	A	565	31.954	8.451	4.406	1.00	43.36	C
ATOM	4431	O	PRO	A	565	32.739	9.117	3.679	1.00	43.41	O
ATOM	4432	N	TRP	A	566	32.372	7.756	5.480	1.00	42.72	N
ATOM	4433	CA	TRP	A	566	33.757	7.880	5.934	1.00	41.56	C
ATOM	4434	CB	TRP	A	566	34.099	6.967	7.143	1.00	41.25	C
ATOM	4435	CG	TRP	A	566	33.744	5.527	7.000	1.00	41.26	C
ATOM	4436	CD1	TRP	A	566	32.583	4.920	7.406	1.00	42.93	C
ATOM	4437	NE1	TRP	A	566	32.618	3.576	7.110	1.00	42.62	N
ATOM	4438	CE2	TRP	A	566	33.815	3.286	6.504	1.00	40.56	C
ATOM	4439	CD2	TRP	A	566	34.549	4.491	6.415	1.00	40.70	C
ATOM	4440	CE3	TRP	A	566	35.813	4.461	5.799	1.00	39.99	C
ATOM	4441	CZ3	TRP	A	566	36.290	3.265	5.309	1.00	37.37	C
ATOM	4442	CH2	TRP	A	566	35.533	2.097	5.417	1.00	37.48	C
ATOM	4443	CZ2	TRP	A	566	34.297	2.084	6.004	1.00	37.86	C
ATOM	4444	C	TRP	A	566	34.553	7.582	4.695	1.00	40.62	C
ATOM	4445	O	TRP	A	566	35.493	8.285	4.347	1.00	39.92	O
ATOM	4446	N	THR	A	567	34.053	6.593	3.979	1.00	39.88	N
ATOM	4447	CA	THR	A	567	34.685	6.130	2.788	1.00	40.19	C
ATOM	4448	CB	THR	A	567	33.906	4.940	2.243	1.00	39.71	C
ATOM	4449	OG1	THR	A	567	33.635	5.132	0.858	1.00	40.03	O
ATOM	4450	CG2	THR	A	567	32.552	4.903	2.887	1.00	38.83	C
ATOM	4451	C	THR	A	567	34.899	7.280	1.794	1.00	40.84	C
ATOM	4452	O	THR	A	567	35.995	7.452	1.252	1.00	40.84	O
ATOM	4453	N	LEU	A	568	33.899	8.116	1.585	1.00	41.82	N
ATOM	4454	CA	LEU	A	568	34.198	9.327	0.836	1.00	43.04	C
ATOM	4455	CB	LEU	A	568	32.946	10.183	0.571	1.00	43.06	C
ATOM	4456	CG	LEU	A	568	33.007	11.176	-0.615	1.00	43.64	C
ATOM	4457	CD1	LEU	A	568	31.601	11.616	-0.876	1.00	45.39	C
ATOM	4458	CD2	LEU	A	568	33.935	12.434	-0.466	1.00	43.99	C
ATOM	4459	C	LEU	A	568	35.268	10.109	1.619	1.00	43.49	C
ATOM	4460	O	LEU	A	568	36.453	10.068	1.280	1.00	42.96	O
ATOM	4461	N	ALA	A	569	34.824	10.773	2.683	1.00	44.34	N
ATOM	4462	CA	ALA	A	569	35.662	11.606	3.534	1.00	45.19	C
ATOM	4463	CB	ALA	A	569	35.108	11.588	4.961	1.00	45.25	C
ATOM	4464	C	ALA	A	569	37.149	11.210	3.511	1.00	45.60	C
ATOM	4465	O	ALA	A	569	37.996	12.026	3.125	1.00	44.83	O
ATOM	4466	N	LEU	A	570	37.434	9.962	3.926	1.00	46.39	N
ATOM	4467	CA	LEU	A	570	38.766	9.354	3.852	1.00	46.91	C
ATOM	4468	CB	LEU	A	570	38.716	7.845	4.104	1.00	46.67	C
ATOM	4469	CG	LEU	A	570	39.782	6.957	4.791	1.00	45.84	C
ATOM	4470	CD1	LEU	A	570	40.343	5.911	3.845	1.00	44.53	C
ATOM	4471	CD2	LEU	A	570	40.921	7.661	5.489	1.00	44.08	C
ATOM	4472	C	LEU	A	570	39.279	9.624	2.465	1.00	47.88	C
ATOM	4473	O	LEU	A	570	40.025	10.589	2.289	1.00	48.11	O
ATOM	4474	N	GLU	A	571	38.833	8.841	1.473	1.00	48.90	N
ATOM	4475	CA	GLU	A	571	39.277	9.042	0.084	1.00	50.30	C
ATOM	4476	CB	GLU	A	571	38.250	8.548	-0.940	1.00	50.63	C
ATOM	4477	CG	GLU	A	571	38.760	8.596	-2.393	1.00	53.24	C

281/396

Figure 3A-81

ATOM	4478	CD	GLU	A	571	37.868	9.389	-3.360	1.00	55.79	C
ATOM	4479	OE1	GLU	A	571	38.173	10.576	-3.667	1.00	54.37	O
ATOM	4480	OE2	GLU	A	571	36.859	8.801	-3.832	1.00	58.11	O
ATOM	4481	C	GLU	A	571	39.551	10.516	-0.173	1.00	50.60	C
ATOM	4482	O	GLU	A	571	40.631	10.906	-0.613	1.00	50.65	O
ATOM	4483	N	ASN	A	572	38.556	11.330	0.144	1.00	51.16	N
ATOM	4484	CA	ASN	A	572	38.628	12.758	-0.062	1.00	51.21	C
ATOM	4485	CB	ASN	A	572	37.299	13.392	0.346	1.00	51.62	C
ATOM	4486	CG	ASN	A	572	37.187	14.801	-0.129	1.00	52.57	C
ATOM	4487	OD1	ASN	A	572	37.046	15.037	-1.338	1.00	52.15	O
ATOM	4488	ND2	ASN	A	572	37.304	15.771	0.810	1.00	53.16	N
ATOM	4489	C	ASN	A	572	39.835	13.512	0.569	1.00	50.73	C
ATOM	4490	O	ASN	A	572	40.240	14.564	0.018	1.00	51.19	O
ATOM	4491	N	VAL	A	573	40.402	13.017	1.691	1.00	49.38	N
ATOM	4492	CA	VAL	A	573	41.621	13.642	2.267	1.00	47.85	C
ATOM	4493	CB	VAL	A	573	41.613	13.779	3.807	1.00	47.32	C
ATOM	4494	CG1	VAL	A	573	42.479	14.890	4.159	1.00	46.73	C
ATOM	4495	CG2	VAL	A	573	40.241	13.998	4.400	1.00	46.13	C
ATOM	4496	C	VAL	A	573	42.847	12.814	1.948	1.00	47.56	C
ATOM	4497	O	VAL	A	573	43.399	12.817	0.849	1.00	47.89	O
ATOM	4498	N	VAL	A	574	43.286	12.128	2.969	1.00	46.92	N
ATOM	4499	CA	VAL	A	574	44.002	10.891	2.833	1.00	46.79	C
ATOM	4500	CB	VAL	A	574	43.806	10.150	4.149	1.00	46.60	C
ATOM	4501	CG1	VAL	A	574	43.781	11.151	5.260	1.00	46.11	C
ATOM	4502	CG2	VAL	A	574	42.494	9.441	4.175	1.00	46.80	C
ATOM	4503	C	VAL	A	574	43.554	10.044	1.597	1.00	47.13	C
ATOM	4504	O	VAL	A	574	42.831	9.042	1.737	1.00	47.12	O
ATOM	4505	N	GLY	A	575	44.010	10.456	0.402	1.00	47.13	N
ATOM	4506	CA	GLY	A	575	43.678	9.859	-0.895	1.00	47.12	C
ATOM	4507	C	GLY	A	575	43.049	8.476	-1.184	1.00	47.24	C
ATOM	4508	O	GLY	A	575	42.897	8.127	-2.349	1.00	47.53	O
ATOM	4509	N	ALA	A	576	42.678	7.665	-0.207	1.00	47.23	N
ATOM	4510	CA	ALA	A	576	42.026	6.409	-0.572	1.00	48.09	C
ATOM	4511	CB	ALA	A	576	42.997	5.246	-0.546	1.00	47.92	C
ATOM	4512	C	ALA	A	576	40.793	6.124	0.285	1.00	48.94	C
ATOM	4513	O	ALA	A	576	40.744	6.514	1.457	1.00	49.30	O
ATOM	4514	N	LYS	A	577	39.797	5.463	-0.317	1.00	49.36	N
ATOM	4515	CA	LYS	A	577	38.508	5.235	0.321	1.00	49.46	C
ATOM	4516	CB	LYS	A	577	37.372	5.149	-0.710	1.00	49.46	C
ATOM	4517	CG	LYS	A	577	37.701	4.541	-2.091	1.00	50.07	C
ATOM	4518	CD	LYS	A	577	36.502	3.704	-2.664	1.00	49.43	C
ATOM	4519	CE	LYS	A	577	36.230	3.921	-4.168	1.00	48.23	C
ATOM	4520	NZ	LYS	A	577	37.081	3.090	-5.100	1.00	46.94	N
ATOM	4521	C	LYS	A	577	38.490	4.030	1.246	1.00	50.00	C
ATOM	4522	O	LYS	A	577	37.438	3.658	1.758	1.00	50.14	O
ATOM	4523	N	ASN	A	578	39.648	3.413	1.470	1.00	50.93	N
ATOM	4524	CA	ASN	A	578	39.728	2.306	2.433	1.00	51.53	C
ATOM	4525	CB	ASN	A	578	39.528	0.957	1.747	1.00	51.44	C
ATOM	4526	CG	ASN	A	578	38.647	0.022	2.570	1.00	52.47	C
ATOM	4527	OD1	ASN	A	578	38.655	0.071	3.811	1.00	52.22	O
ATOM	4528	ND2	ASN	A	578	37.880	-0.840	1.886	1.00	54.52	N
ATOM	4529	C	ASN	A	578	40.959	2.270	3.353	1.00	51.62	C
ATOM	4530	O	ASN	A	578	41.945	2.946	3.102	1.00	51.91	O
ATOM	4531	N	MET	A	579	40.857	1.500	4.434	1.00	51.54	N
ATOM	4532	CA	MET	A	579	41.915	1.304	5.410	1.00	51.53	C
ATOM	4533	CB	MET	A	579	41.507	0.176	6.315	1.00	51.67	C

282/396

Figure 3A-82

ATOM	4534	CG	MET	A	579	41.257	0.593	7.703	1.00	53.94	C
ATOM	4535	SD	MET	A	579	41.309	-0.892	8.730	1.00	61.09	S
ATOM	4536	CE	MET	A	579	39.770	-1.914	8.050	1.00	60.10	C
ATOM	4537	C	MET	A	579	43.280	0.942	4.836	1.00	51.38	C
ATOM	4538	O	MET	A	579	43.435	-0.065	4.133	1.00	51.38	O
ATOM	4539	N	ASN	A	580	44.283	1.746	5.172	1.00	51.20	N
ATOM	4540	CA	ASN	A	580	45.646	1.449	4.755	1.00	51.00	C
ATOM	4541	CB	ASN	A	580	46.245	2.592	3.933	1.00	51.90	C
ATOM	4542	CG	ASN	A	580	47.201	2.092	2.864	1.00	54.72	C
ATOM	4543	OD1	ASN	A	580	47.810	2.890	2.104	1.00	56.80	O
ATOM	4544	ND2	ASN	A	580	47.334	0.749	2.784	1.00	56.27	N
ATOM	4545	C	ASN	A	580	46.603	1.097	5.872	1.00	49.80	C
ATOM	4546	O	ASN	A	580	46.839	1.940	6.778	1.00	49.25	O
ATOM	4547	N	VAL	A	581	47.134	-0.145	5.781	1.00	48.57	N
ATOM	4548	CA	VAL	A	581	48.232	-0.650	6.638	1.00	46.78	C
ATOM	4549	CB	VAL	A	581	48.263	-2.174	6.784	1.00	45.79	C
ATOM	4550	CG1	VAL	A	581	49.339	-2.759	5.918	1.00	43.76	C
ATOM	4551	CG2	VAL	A	581	48.470	-2.549	8.239	1.00	42.92	C
ATOM	4552	C	VAL	A	581	49.527	-0.195	6.032	1.00	47.12	C
ATOM	4553	O	VAL	A	581	50.510	0.095	6.727	1.00	46.81	O
ATOM	4554	N	ARG	A	582	49.479	-0.054	4.724	1.00	47.15	N
ATOM	4555	CA	ARG	A	582	50.669	0.220	3.962	1.00	48.26	C
ATOM	4556	CB	ARG	A	582	50.336	0.154	2.453	1.00	49.14	C
ATOM	4557	CG	ARG	A	582	50.087	-1.299	1.892	1.00	52.62	C
ATOM	4558	CD	ARG	A	582	48.634	-1.700	1.419	1.00	57.17	C
ATOM	4559	NE	ARG	A	582	48.151	-1.005	0.214	1.00	58.60	N
ATOM	4560	CZ	ARG	A	582	47.904	-1.590	-0.953	1.00	58.93	C
ATOM	4561	NH1	ARG	A	582	48.123	-2.896	-1.118	1.00	59.70	N
ATOM	4562	NH2	ARG	A	582	47.467	-0.854	-1.968	1.00	58.21	N
ATOM	4563	C	ARG	A	582	51.567	1.448	4.346	1.00	47.49	C
ATOM	4564	O	ARG	A	582	52.652	1.541	3.820	1.00	47.27	O
ATOM	4565	N	PRO	A	583	51.159	2.404	5.177	1.00	47.14	N
ATOM	4566	CA	PRO	A	583	52.143	3.344	5.729	1.00	47.42	C
ATOM	4567	CB	PRO	A	583	51.462	4.715	5.552	1.00	47.50	C
ATOM	4568	CG	PRO	A	583	49.971	4.375	5.465	1.00	47.94	C
ATOM	4569	CD	PRO	A	583	49.794	2.832	5.507	1.00	47.24	C
ATOM	4570	C	PRO	A	583	52.501	3.131	7.204	1.00	47.57	C
ATOM	4571	O	PRO	A	583	53.528	3.650	7.661	1.00	47.58	O
ATOM	4572	N	LEU	A	584	51.674	2.410	7.952	1.00	47.43	N
ATOM	4573	CA	LEU	A	584	52.041	2.093	9.325	1.00	47.63	C
ATOM	4574	CB	LEU	A	584	50.828	1.601	10.118	1.00	47.58	C
ATOM	4575	CG	LEU	A	584	50.915	0.716	11.373	1.00	47.16	C
ATOM	4576	CD1	LEU	A	584	49.779	1.053	12.324	1.00	46.95	C
ATOM	4577	CD2	LEU	A	584	50.902	-0.781	11.042	1.00	44.60	C
ATOM	4578	C	LEU	A	584	53.133	1.020	9.251	1.00	48.11	C
ATOM	4579	O	LEU	A	584	53.583	0.497	10.286	1.00	48.92	O
ATOM	4580	N	LEU	A	585	53.528	0.672	8.015	1.00	47.67	N
ATOM	4581	CA	LEU	A	585	54.687	-0.188	7.743	1.00	46.26	C
ATOM	4582	CB	LEU	A	585	54.405	-1.161	6.618	1.00	45.03	C
ATOM	4583	CG	LEU	A	585	53.954	-2.515	7.133	1.00	43.15	C
ATOM	4584	CD1	LEU	A	585	53.208	-2.454	8.427	1.00	40.14	C
ATOM	4585	CD2	LEU	A	585	53.100	-3.164	6.103	1.00	44.44	C
ATOM	4586	C	LEU	A	585	55.809	0.737	7.382	1.00	46.50	C
ATOM	4587	O	LEU	A	585	56.813	0.776	8.047	1.00	46.58	O
ATOM	4588	N	ASN	A	586	55.614	1.516	6.341	1.00	47.05	N
ATOM	4589	CA	ASN	A	586	56.478	2.634	6.102	1.00	48.13	C

283/396

Figure 3A-83

ATOM	4590	CB	ASN	A	586	55.775	3.675	5.232	1.00	48.65	C
ATOM	4591	CG	ASN	A	586	55.923	3.384	3.741	1.00	50.96	C
ATOM	4592	OD1	ASN	A	586	55.551	4.233	2.877	1.00	53.54	O
ATOM	4593	ND2	ASN	A	586	56.457	2.172	3.414	1.00	50.18	N
ATOM	4594	C	ASN	A	586	56.972	3.265	7.405	1.00	48.29	C
ATOM	4595	O	ASN	A	586	58.165	3.143	7.726	1.00	48.76	O
ATOM	4596	N	TYR	A	587	56.078	3.919	8.158	1.00	48.02	N
ATOM	4597	CA	TYR	A	587	56.507	4.738	9.305	1.00	47.28	C
ATOM	4598	CB	TYR	A	587	55.303	5.330	10.068	1.00	47.25	C
ATOM	4599	CG	TYR	A	587	55.525	6.024	11.434	1.00	45.56	C
ATOM	4600	CD1	TYR	A	587	55.198	7.358	11.617	1.00	44.72	C
ATOM	4601	CE1	TYR	A	587	55.357	7.966	12.838	1.00	43.35	C
ATOM	4602	CZ	TYR	A	587	55.819	7.235	13.902	1.00	42.96	C
ATOM	4603	OH	TYR	A	587	55.971	7.818	15.127	1.00	43.82	O
ATOM	4604	CE2	TYR	A	587	56.124	5.920	13.762	1.00	42.61	C
ATOM	4605	CD2	TYR	A	587	55.956	5.317	12.547	1.00	43.86	C
ATOM	4606	C	TYR	A	587	57.407	3.888	10.171	1.00	47.19	C
ATOM	4607	O	TYR	A	587	58.309	4.400	10.802	1.00	47.77	O
ATOM	4608	N	PHE	A	588	57.213	2.581	10.136	1.00	46.76	N
ATOM	4609	CA	PHE	A	588	58.048	1.696	10.924	1.00	47.01	C
ATOM	4610	CB	PHE	A	588	57.168	0.629	11.575	1.00	47.01	C
ATOM	4611	CG	PHE	A	588	56.426	1.086	12.785	1.00	45.00	C
ATOM	4612	CD1	PHE	A	588	55.573	0.216	13.429	1.00	43.08	C
ATOM	4613	CE1	PHE	A	588	54.889	0.609	14.536	1.00	41.47	C
ATOM	4614	CZ	PHE	A	588	55.031	1.863	15.008	1.00	41.97	C
ATOM	4615	CE2	PHE	A	588	55.883	2.739	14.387	1.00	42.73	C
ATOM	4616	CD2	PHE	A	588	56.577	2.355	13.284	1.00	43.11	C
ATOM	4617	C	PHE	A	588	59.190	0.961	10.182	1.00	47.65	C
ATOM	4618	O	PHE	A	588	59.937	0.229	10.824	1.00	48.16	O
ATOM	4619	N	GLU	A	589	59.330	1.091	8.864	1.00	47.82	N
ATOM	4620	CA	GLU	A	589	60.327	0.259	8.187	1.00	48.11	C
ATOM	4621	CB	GLU	A	589	60.299	0.361	6.661	1.00	48.28	C
ATOM	4622	CG	GLU	A	589	58.963	-0.063	6.033	1.00	51.82	C
ATOM	4623	CD	GLU	A	589	58.730	-1.589	5.872	1.00	55.51	C
ATOM	4624	OE1	GLU	A	589	57.889	-2.165	6.635	1.00	54.78	O
ATOM	4625	OE2	GLU	A	589	59.344	-2.208	4.944	1.00	56.19	O
ATOM	4626	C	GLU	A	589	61.733	0.437	8.761	1.00	47.77	C
ATOM	4627	O	GLU	A	589	62.396	-0.570	8.985	1.00	48.32	O
ATOM	4628	N	PRO	A	590	62.180	1.671	9.029	1.00	47.13	N
ATOM	4629	CA	PRO	A	590	63.430	1.912	9.756	1.00	46.66	C
ATOM	4630	CB	PRO	A	590	63.215	3.293	10.347	1.00	46.67	C
ATOM	4631	CG	PRO	A	590	62.441	3.972	9.344	1.00	47.36	C
ATOM	4632	CD	PRO	A	590	61.569	2.945	8.630	1.00	47.33	C
ATOM	4633	C	PRO	A	590	63.670	0.916	10.870	1.00	46.37	C
ATOM	4634	O	PRO	A	590	64.413	-0.049	10.633	1.00	47.08	O
ATOM	4635	N	LEU	A	591	63.066	1.124	12.041	1.00	45.54	N
ATOM	4636	CA	LEU	A	591	63.164	0.148	13.133	1.00	44.93	C
ATOM	4637	CB	LEU	A	591	62.503	0.673	14.426	1.00	44.85	C
ATOM	4638	CG	LEU	A	591	61.496	-0.206	15.212	1.00	45.03	C
ATOM	4639	CD1	LEU	A	591	62.088	-0.910	16.449	1.00	43.83	C
ATOM	4640	CD2	LEU	A	591	60.310	0.607	15.611	1.00	44.73	C
ATOM	4641	C	LEU	A	591	62.655	-1.272	12.756	1.00	44.59	C
ATOM	4642	O	LEU	A	591	62.980	-2.245	13.437	1.00	44.71	O
ATOM	4643	N	PHE	A	592	61.875	-1.415	11.689	1.00	43.86	N
ATOM	4644	CA	PHE	A	592	61.483	-2.750	11.337	1.00	43.55	C
ATOM	4645	CB	PHE	A	592	60.520	-2.819	10.160	1.00	43.27	C

284/396

Figure 3A-84

ATOM	4646	CG	PHE	A	592	60.226	-4.248	9.668	1.00	41.40	C
ATOM	4647	CD1	PHE	A	592	59.709	-5.212	10.527	1.00	40.47	C
ATOM	4648	CE1	PHE	A	592	59.436	-6.499	10.057	1.00	39.33	C
ATOM	4649	CZ	PHE	A	592	59.656	-6.811	8.719	1.00	37.02	C
ATOM	4650	CE2	PHE	A	592	60.160	-5.865	7.862	1.00	35.54	C
ATOM	4651	CD2	PHE	A	592	60.444	-4.606	8.331	1.00	38.05	C
ATOM	4652	C	PHE	A	592	62.759	-3.459	11.011	1.00	44.45	C
ATOM	4653	O	PHE	A	592	62.999	-4.499	11.609	1.00	45.22	O
ATOM	4654	N	THR	A	593	63.593	-2.889	10.115	1.00	44.93	N
ATOM	4655	CA	THR	A	593	64.814	-3.570	9.579	1.00	45.06	C
ATOM	4656	CB	THR	A	593	65.397	-2.840	8.329	1.00	44.68	C
ATOM	4657	OG1	THR	A	593	64.665	-1.646	8.067	1.00	44.19	O
ATOM	4658	CG2	THR	A	593	65.176	-3.651	7.071	1.00	44.00	C
ATOM	4659	C	THR	A	593	65.929	-3.785	10.618	1.00	45.71	C
ATOM	4660	O	THR	A	593	66.462	-4.899	10.770	1.00	44.60	O
ATOM	4661	N	TRP	A	594	66.272	-2.710	11.328	1.00	46.74	N
ATOM	4662	CA	TRP	A	594	67.179	-2.807	12.451	1.00	48.49	C
ATOM	4663	CB	TRP	A	594	67.352	-1.430	13.065	1.00	48.42	C
ATOM	4664	CG	TRP	A	594	67.968	-1.340	14.484	1.00	50.66	C
ATOM	4665	CD1	TRP	A	594	69.064	-0.580	14.865	1.00	51.90	C
ATOM	4666	NE1	TRP	A	594	69.281	-0.712	16.218	1.00	52.46	N
ATOM	4667	CE2	TRP	A	594	68.335	-1.551	16.751	1.00	50.55	C
ATOM	4668	CD2	TRP	A	594	67.483	-1.960	15.700	1.00	50.27	C
ATOM	4669	CE3	TRP	A	594	66.405	-2.805	16.004	1.00	47.73	C
ATOM	4670	CZ3	TRP	A	594	66.235	-3.219	17.277	1.00	47.11	C
ATOM	4671	CH2	TRP	A	594	67.093	-2.798	18.296	1.00	48.73	C
ATOM	4672	CZ2	TRP	A	594	68.145	-1.960	18.053	1.00	49.36	C
ATOM	4673	C	TRP	A	594	66.691	-3.840	13.480	1.00	49.47	C
ATOM	4674	O	TRP	A	594	67.418	-4.188	14.418	1.00	49.82	O
ATOM	4675	N	LEU	A	595	65.470	-4.336	13.291	1.00	50.61	N
ATOM	4676	CA	LEU	A	595	64.867	-5.313	14.192	1.00	51.54	C
ATOM	4677	CB	LEU	A	595	63.383	-5.049	14.381	1.00	51.41	C
ATOM	4678	CG	LEU	A	595	62.929	-5.447	15.779	1.00	52.10	C
ATOM	4679	CD1	LEU	A	595	62.963	-4.239	16.721	1.00	52.43	C
ATOM	4680	CD2	LEU	A	595	61.555	-6.048	15.713	1.00	51.72	C
ATOM	4681	C	LEU	A	595	65.025	-6.714	13.707	1.00	52.33	C
ATOM	4682	O	LEU	A	595	64.994	-7.624	14.494	1.00	52.18	O
ATOM	4683	N	LYS	A	596	65.145	-6.898	12.403	1.00	54.18	N
ATOM	4684	CA	LYS	A	596	65.456	-8.225	11.872	1.00	55.62	C
ATOM	4685	CB	LYS	A	596	64.876	-8.474	10.467	1.00	55.61	C
ATOM	4686	CG	LYS	A	596	63.684	-7.665	10.000	1.00	53.18	C
ATOM	4687	CD	LYS	A	596	63.182	-8.299	8.701	1.00	52.46	C
ATOM	4688	CE	LYS	A	596	64.121	-8.146	7.453	1.00	51.23	C
ATOM	4689	NZ	LYS	A	596	64.234	-6.775	6.796	1.00	47.89	N
ATOM	4690	C	LYS	A	596	66.973	-8.471	11.845	1.00	57.06	C
ATOM	4691	O	LYS	A	596	67.402	-9.620	11.664	1.00	56.88	O
ATOM	4692	N	ASP	A	597	67.765	-7.388	11.978	1.00	58.73	N
ATOM	4693	CA	ASP	A	597	69.200	-7.492	12.313	1.00	60.10	C
ATOM	4694	CB	ASP	A	597	69.983	-6.175	12.080	1.00	60.75	C
ATOM	4695	CG	ASP	A	597	70.783	-6.159	10.714	1.00	65.07	C
ATOM	4696	OD1	ASP	A	597	71.358	-7.224	10.307	1.00	67.68	O
ATOM	4697	OD2	ASP	A	597	70.888	-5.118	9.977	1.00	68.42	O
ATOM	4698	C	ASP	A	597	69.225	-7.882	13.770	1.00	59.60	C
ATOM	4699	O	ASP	A	597	69.133	-9.056	14.111	1.00	59.08	O
ATOM	4700	N	GLN	A	598	69.259	-6.874	14.622	1.00	59.78	N
ATOM	4701	CA	GLN	A	598	69.203	-7.053	16.068	1.00	60.00	C

285/396

Figure 3A-85

ATOM	4702	CB	GLN	A	598	68.675	-5.774	16.710	1.00	60.05	C
ATOM	4703	CG	GLN	A	598	69.775	-4.791	17.005	1.00	60.45	C
ATOM	4704	CD	GLN	A	598	70.385	-5.046	18.373	1.00	61.95	C
ATOM	4705	OE1	GLN	A	598	70.119	-6.083	18.998	1.00	61.67	O
ATOM	4706	NE2	GLN	A	598	71.185	-4.094	18.857	1.00	62.73	N
ATOM	4707	C	GLN	A	598	68.465	-8.283	16.608	1.00	59.91	C
ATOM	4708	O	GLN	A	598	68.573	-8.584	17.789	1.00	59.77	O
ATOM	4709	N	ASN	A	599	67.763	-9.007	15.740	1.00	60.20	N
ATOM	4710	CA	ASN	A	599	67.044	-10.223	16.131	1.00	60.92	C
ATOM	4711	CB	ASN	A	599	65.615	-10.247	15.540	1.00	60.88	C
ATOM	4712	CG	ASN	A	599	64.525	-9.825	16.537	1.00	59.25	C
ATOM	4713	OD1	ASN	A	599	63.694	-10.624	16.943	1.00	56.59	O
ATOM	4714	ND2	ASN	A	599	64.508	-8.552	16.882	1.00	59.07	N
ATOM	4715	C	ASN	A	599	67.760	-11.476	15.659	1.00	61.74	C
ATOM	4716	O	ASN	A	599	67.423	-12.574	16.118	1.00	61.18	O
ATOM	4717	N	LYS	A	600	68.714	-11.281	14.730	1.00	63.12	N
ATOM	4718	CA	LYS	A	600	69.482	-12.318	13.982	1.00	64.49	C
ATOM	4719	CB	LYS	A	600	70.972	-11.979	13.999	1.00	64.48	C
ATOM	4720	CG	LYS	A	600	71.380	-10.698	13.335	1.00	66.02	C
ATOM	4721	CD	LYS	A	600	72.795	-10.270	13.799	1.00	68.21	C
ATOM	4722	CE	LYS	A	600	73.350	-9.200	12.865	1.00	69.97	C
ATOM	4723	NZ	LYS	A	600	72.897	-9.403	11.424	1.00	71.49	N
ATOM	4724	C	LYS	A	600	69.384	-13.748	14.504	1.00	65.20	C
ATOM	4725	O	LYS	A	600	69.216	-14.727	13.748	1.00	65.21	O
ATOM	4726	N	ASN	A	601	69.506	-13.813	15.824	1.00	66.06	N
ATOM	4727	CA	ASN	A	601	69.735	-15.001	16.632	1.00	66.94	C
ATOM	4728	CB	ASN	A	601	70.655	-14.554	17.763	1.00	67.37	C
ATOM	4729	CG	ASN	A	601	70.500	-13.065	18.057	1.00	69.61	C
ATOM	4730	OD1	ASN	A	601	69.862	-12.687	19.051	1.00	72.51	O
ATOM	4731	ND2	ASN	A	601	71.044	-12.205	17.166	1.00	70.51	N
ATOM	4732	C	ASN	A	601	68.441	-15.566	17.237	1.00	66.74	C
ATOM	4733	O	ASN	A	601	68.099	-16.752	17.013	1.00	66.56	O
ATOM	4734	N	SER	A	602	67.738	-14.694	17.986	1.00	66.29	N
ATOM	4735	CA	SER	A	602	66.494	-15.013	18.714	1.00	65.58	C
ATOM	4736	CB	SER	A	602	65.997	-13.781	19.534	1.00	65.72	C
ATOM	4737	OG	SER	A	602	65.753	-14.058	20.924	1.00	65.39	O
ATOM	4738	C	SER	A	602	65.408	-15.527	17.752	1.00	64.74	C
ATOM	4739	O	SER	A	602	65.384	-15.157	16.568	1.00	64.79	O
ATOM	4740	N	PHE	A	603	64.531	-16.390	18.256	1.00	63.51	N
ATOM	4741	CA	PHE	A	603	63.416	-16.863	17.471	1.00	62.68	C
ATOM	4742	CB	PHE	A	603	62.602	-17.818	18.294	1.00	61.94	C
ATOM	4743	CG	PHE	A	603	61.661	-18.626	17.492	1.00	61.04	C
ATOM	4744	CD1	PHE	A	603	60.779	-19.499	18.116	1.00	61.50	C
ATOM	4745	CE1	PHE	A	603	59.901	-20.279	17.381	1.00	61.58	C
ATOM	4746	CZ	PHE	A	603	59.906	-20.187	15.986	1.00	62.60	C
ATOM	4747	CE2	PHE	A	603	60.790	-19.303	15.351	1.00	62.36	C
ATOM	4748	CD2	PHE	A	603	61.659	-18.538	16.110	1.00	60.77	C
ATOM	4749	C	PHE	A	603	62.516	-15.708	17.057	1.00	63.07	C
ATOM	4750	O	PHE	A	603	62.252	-14.824	17.868	1.00	63.56	O
ATOM	4751	N	VAL	A	604	62.062	-15.709	15.798	1.00	63.18	N
ATOM	4752	CA	VAL	A	604	60.999	-14.801	15.319	1.00	62.90	C
ATOM	4753	CB	VAL	A	604	61.409	-14.042	14.002	1.00	62.82	C
ATOM	4754	CG1	VAL	A	604	60.204	-13.602	13.172	1.00	62.65	C
ATOM	4755	CG2	VAL	A	604	62.260	-12.840	14.337	1.00	62.09	C
ATOM	4756	C	VAL	A	604	59.691	-15.608	15.192	1.00	63.11	C
ATOM	4757	O	VAL	A	604	59.505	-16.385	14.241	1.00	62.80	O

286/396

Figure 3A-86

ATOM	4758	N	GLY	A	605	58.811	-15.436	16.182	1.00	63.28	N
ATOM	4759	CA	GLY	A	605	57.652	-16.295	16.349	1.00	63.75	C
ATOM	4760	C	GLY	A	605	57.529	-16.866	17.743	1.00	64.16	C
ATOM	4761	O	GLY	A	605	58.249	-16.462	18.645	1.00	63.49	O
ATOM	4762	N	TRP	A	606	56.607	-17.811	17.911	1.00	65.60	N
ATOM	4763	CA	TRP	A	606	56.288	-18.386	19.231	1.00	67.34	C
ATOM	4764	CB	TRP	A	606	55.492	-17.387	20.112	1.00	67.54	C
ATOM	4765	CG	TRP	A	606	54.103	-17.024	19.563	1.00	68.78	C
ATOM	4766	CD1	TRP	A	606	53.004	-17.860	19.395	1.00	70.30	C
ATOM	4767	NE1	TRP	A	606	51.949	-17.160	18.855	1.00	69.28	N
ATOM	4768	CE2	TRP	A	606	52.344	-15.865	18.660	1.00	68.27	C
ATOM	4769	CD2	TRP	A	606	53.690	-15.747	19.100	1.00	67.91	C
ATOM	4770	CE3	TRP	A	606	54.323	-14.514	18.994	1.00	66.64	C
ATOM	4771	CZ3	TRP	A	606	53.634	-13.467	18.493	1.00	68.67	C
ATOM	4772	CH2	TRP	A	606	52.295	-13.606	18.075	1.00	69.92	C
ATOM	4773	CZ2	TRP	A	606	51.640	-14.802	18.148	1.00	69.01	C
ATOM	4774	C	TRP	A	606	55.535	-19.728	19.221	1.00	68.08	C
ATOM	4775	O	TRP	A	606	54.938	-20.136	18.208	1.00	67.46	O
ATOM	4776	N	SER	A	607	55.548	-20.363	20.396	1.00	69.54	N
ATOM	4777	CA	SER	A	607	54.824	-21.598	20.662	1.00	71.16	C
ATOM	4778	CB	SER	A	607	55.738	-22.630	21.282	1.00	70.80	C
ATOM	4779	OG	SER	A	607	55.106	-23.889	21.203	1.00	71.47	O
ATOM	4780	C	SER	A	607	53.555	-21.477	21.523	1.00	72.41	C
ATOM	4781	O	SER	A	607	53.511	-20.762	22.529	1.00	72.43	O
ATOM	4782	N	THR	A	608	52.549	-22.244	21.108	1.00	74.14	N
ATOM	4783	CA	THR	A	608	51.193	-22.222	21.644	1.00	75.76	C
ATOM	4784	CB	THR	A	608	50.147	-22.286	20.451	1.00	75.96	C
ATOM	4785	OG1	THR	A	608	49.125	-23.268	20.705	1.00	76.50	O
ATOM	4786	CG2	THR	A	608	50.799	-22.788	19.133	1.00	75.65	C
ATOM	4787	C	THR	A	608	50.969	-23.368	22.656	1.00	76.70	C
ATOM	4788	O	THR	A	608	49.832	-23.594	23.113	1.00	77.06	O
ATOM	4789	N	ASP	A	609	52.047	-24.078	23.006	1.00	77.44	N
ATOM	4790	CA	ASP	A	609	51.951	-25.294	23.820	1.00	78.18	C
ATOM	4791	CB	ASP	A	609	52.788	-26.425	23.199	1.00	78.24	C
ATOM	4792	CG	ASP	A	609	52.179	-26.996	21.922	1.00	77.93	C
ATOM	4793	OD1	ASP	A	609	52.337	-26.370	20.843	1.00	77.57	O
ATOM	4794	OD2	ASP	A	609	51.555	-28.081	21.906	1.00	76.75	O
ATOM	4795	C	ASP	A	609	52.457	-25.035	25.227	1.00	78.79	C
ATOM	4796	O	ASP	A	609	52.065	-25.714	26.172	1.00	78.74	O
ATOM	4797	N	TRP	A	610	53.336	-24.046	25.333	1.00	79.68	N
ATOM	4798	CA	TRP	A	610	54.142	-23.742	26.518	1.00	80.77	C
ATOM	4799	CB	TRP	A	610	54.874	-22.426	26.249	1.00	80.95	C
ATOM	4800	CG	TRP	A	610	55.939	-22.051	27.226	1.00	80.67	C
ATOM	4801	CD1	TRP	A	610	57.052	-22.762	27.542	1.00	80.83	C
ATOM	4802	NE1	TRP	A	610	57.800	-22.082	28.468	1.00	80.48	N
ATOM	4803	CE2	TRP	A	610	57.173	-20.902	28.754	1.00	81.32	C
ATOM	4804	CD2	TRP	A	610	56.000	-20.854	27.980	1.00	81.05	C
ATOM	4805	CE3	TRP	A	610	55.166	-19.739	28.098	1.00	83.28	C
ATOM	4806	CZ3	TRP	A	610	55.534	-18.710	28.975	1.00	84.85	C
ATOM	4807	CH2	TRP	A	610	56.714	-18.794	29.731	1.00	84.34	C
ATOM	4808	CZ2	TRP	A	610	57.541	-19.881	29.634	1.00	82.88	C
ATOM	4809	C	TRP	A	610	53.413	-23.610	27.857	1.00	81.64	C
ATOM	4810	O	TRP	A	610	52.264	-24.050	28.014	1.00	81.70	O
ATOM	4811	N	SER	A	611	54.138	-23.007	28.812	1.00	82.56	N
ATOM	4812	CA	SER	A	611	53.655	-22.551	30.128	1.00	83.31	C
ATOM	4813	CB	SER	A	611	52.962	-23.681	30.923	1.00	83.36	C

287/396

Figure 3A-87

ATOM	4814	OG	SER	A	611	52.610	-23.254	32.235	1.00	82.69	O
ATOM	4815	C	SER	A	611	54.821	-21.987	30.959	1.00	83.78	C
ATOM	4816	O	SER	A	611	55.988	-22.371	30.752	1.00	83.83	O
ATOM	4817	N	PRO	A	612	54.504	-21.070	31.876	1.00	84.01	N
ATOM	4818	CA	PRO	A	612	55.386	-20.743	33.011	1.00	84.30	C
ATOM	4819	CB	PRO	A	612	55.096	-19.265	33.242	1.00	84.29	C
ATOM	4820	CG	PRO	A	612	53.684	-19.060	32.706	1.00	84.25	C
ATOM	4821	CD	PRO	A	612	53.302	-20.221	31.842	1.00	83.78	C
ATOM	4822	C	PRO	A	612	55.115	-21.571	34.306	1.00	84.63	C
ATOM	4823	O	PRO	A	612	55.539	-21.192	35.415	1.00	84.59	O
ATOM	4824	N	TYR	A	613	54.425	-22.703	34.149	1.00	84.93	N
ATOM	4825	CA	TYR	A	613	54.083	-23.596	35.262	1.00	85.08	C
ATOM	4826	CB	TYR	A	613	52.939	-22.999	36.099	1.00	85.10	C
ATOM	4827	CG	TYR	A	613	51.755	-22.544	35.270	1.00	84.81	C
ATOM	4828	CD1	TYR	A	613	50.731	-23.432	34.928	1.00	84.47	C
ATOM	4829	CE1	TYR	A	613	49.645	-23.013	34.156	1.00	83.49	C
ATOM	4830	CZ	TYR	A	613	49.579	-21.699	33.731	1.00	82.90	C
ATOM	4831	OH	TYR	A	613	48.519	-21.284	32.984	1.00	82.71	O
ATOM	4832	CE2	TYR	A	613	50.580	-20.809	34.048	1.00	83.17	C
ATOM	4833	CD2	TYR	A	613	51.660	-21.226	34.817	1.00	84.26	C
ATOM	4834	C	TYR	A	613	53.717	-25.016	34.774	1.00	85.16	C
ATOM	4835	O	TYR	A	613	52.801	-25.215	33.960	1.00	84.83	O
ATOM	4836	ZN	ZN	T	1	39.170	7.818	22.095	1.00	62.03	ZN
ATOM	5246	CL	CL	C	999	43.608	-10.834	30.495	1.00	64.57	CCL
ATOM	5217	O1	XX5	Z	500	38.435	7.315	23.786	1.00	25.00	ZO
ATOM	5218	C2	XX5	Z	500	38.637	7.326	25.003	1.00	25.00	ZC
ATOM	5219	O3	XX5	Z	500	38.696	8.382	25.641	1.00	25.00	ZO
ATOM	5220	C4	XX5	Z	500	38.793	5.974	25.743	1.00	25.00	ZC
ATOM	5221	C5	XX5	Z	500	37.436	5.521	26.291	1.00	25.00	ZC
ATOM	5222	C6	XX5	Z	500	36.285	6.488	26.010	1.00	25.00	ZC
ATOM	5223	C7	XX5	Z	500	34.951	5.948	26.525	1.00	25.00	ZC
ATOM	5224	C8	XX5	Z	500	36.206	6.908	24.540	1.00	25.00	ZC
ATOM	5225	N9	XX5	Z	500	39.771	5.998	26.833	1.00	25.00	ZN
ATOM	5226	C10	XX5	Z	500	41.044	5.312	26.588	1.00	25.00	ZC
ATOM	5227	C11	XX5	Z	500	40.946	3.773	26.488	1.00	25.00	ZC
ATOM	5228	O12	XX5	Z	500	41.501	3.209	25.542	1.00	25.00	ZO
ATOM	5229	O13	XX5	Z	500	40.350	3.145	27.366	1.00	25.00	ZO
ATOM	5230	C14	XX5	Z	500	42.092	5.684	27.646	1.00	25.00	ZC
ATOM	5231	C15	XX5	Z	500	43.464	5.681	27.021	1.00	25.00	ZC
ATOM	5232	C16	XX5	Z	500	43.784	6.098	25.717	1.00	25.00	ZC
ATOM	5233	N17	XX5	Z	500	45.113	5.938	25.558	1.00	25.00	ZN
ATOM	5234	C18	XX5	Z	500	45.552	5.405	26.707	1.00	25.00	ZC
ATOM	5235	N19	XX5	Z	500	44.602	5.268	27.653	1.00	25.00	ZN
ATOM	5236	C20	XX5	Z	500	44.714	4.786	29.049	1.00	25.00	ZC
ATOM	5237	C21	XX5	Z	500	46.049	4.245	29.522	1.00	25.00	ZC
ATOM	5238	C22	XX5	Z	500	46.082	3.369	30.604	1.00	25.00	ZC
ATOM	5239	C23	XX5	Z	500	47.289	2.879	31.093	1.00	25.00	ZC
ATOM	5240	CL24	XX5	Z	500	47.326	1.810	32.511	1.00	25.00	ZCL
ATOM	5241	C25	XX5	Z	500	48.483	3.245	30.487	1.00	25.00	ZC
ATOM	5242	C26	XX5	Z	500	47.262	4.634	28.956	1.00	25.00	ZC
ATOM	5243	C27	XX5	Z	500	48.467	4.120	29.412	1.00	25.00	ZC
ATOM	5244	CL28	XX5	Z	500	49.989	4.589	28.630	1.00	25.00	ZCL
ATOM	4889	O	HOH	W	1	43.220	-11.292	30.506	1.00	2.27	O
ATOM	4890	O	HOH	W	2	31.362	8.569	26.752	1.00	9.96	O
ATOM	4891	O	HOH	W	3	44.019	-9.390	28.848	1.00	18.95	O
ATOM	4892	O	HOH	W	4	9.672	-2.614	15.760	1.00	24.41	O

288/396

Figure 3A-88

ATOM	4893	O	HOH	W	5	31.887	23.122	28.416	1.00	38.30	O
ATOM	4894	O	HOH	W	6	43.627	32.519	23.916	1.00	14.90	O
ATOM	4895	O	HOH	W	7	42.525	4.520	34.746	1.00	7.91	O
ATOM	4896	O	HOH	W	8	52.798	6.035	34.614	1.00	6.17	O
ATOM	4897	O	HOH	W	9	54.838	15.029	-1.246	1.00	4.97	O
ATOM	4898	O	HOH	W	10	8.714	-4.330	17.784	1.00	32.07	O
ATOM	4899	O	HOH	W	11	46.005	0.204	29.338	1.00	9.24	O
ATOM	4900	O	HOH	W	12	39.464	4.154	28.356	1.00	7.62	O
ATOM	4901	O	HOH	W	13	41.420	-9.261	48.166	1.00	20.70	O
ATOM	4902	O	HOH	W	14	70.559	-4.209	21.250	1.00	14.02	O
ATOM	4903	O	HOH	W	15	64.027	14.897	15.684	1.00	31.72	O
ATOM	4904	O	HOH	W	16	56.491	-1.599	43.611	1.00	22.60	O
ATOM	4905	O	HOH	W	17	34.793	23.734	17.118	1.00	13.58	O
ATOM	4906	O	HOH	W	18	16.774	12.041	38.140	1.00	60.22	O
ATOM	4907	O	HOH	W	19	8.518	18.797	-0.585	1.00	51.32	O
ATOM	4908	O	HOH	W	20	39.776	22.261	36.505	1.00	42.16	O
ATOM	4909	O	HOH	W	21	45.323	6.702	29.670	1.00	6.74	O
ATOM	4910	O	HOH	W	22	50.635	7.211	35.137	1.00	50.77	O
ATOM	4911	O	HOH	W	23	26.760	14.700	44.658	1.00	31.76	O
ATOM	4912	O	HOH	W	24	64.824	-16.440	21.769	1.00	66.45	O
ATOM	4913	O	HOH	W	25	68.720	-6.098	23.060	1.00	51.53	O
ATOM	4914	O	HOH	W	26	7.638	-1.757	13.750	1.00	53.11	O
ATOM	4915	O	HOH	W	27	58.166	-4.701	32.917	1.00	31.95	O
ATOM	4916	O	HOH	W	28	30.050	0.914	-3.527	1.00	37.02	O
ATOM	4917	O	HOH	W	29	28.528	25.343	14.824	1.00	51.75	O
ATOM	4918	O	HOH	W	30	17.425	21.199	4.372	1.00	16.90	O
ATOM	4919	O	HOH	W	31	57.588	22.290	28.757	1.00	42.28	O
ATOM	4920	O	HOH	W	32	37.080	-24.450	18.041	1.00	48.30	O
ATOM	4921	O	HOH	W	33	67.378	14.464	13.877	1.00	32.27	O
ATOM	4922	O	HOH	W	34	72.679	-0.892	23.140	1.00	35.82	O
ATOM	4923	O	HOH	W	35	39.543	3.221	30.753	1.00	27.26	O
ATOM	4924	O	HOH	W	36	28.427	18.731	19.459	1.00	21.28	O
ATOM	4925	O	HOH	W	37	8.782	-0.926	17.033	1.00	25.84	O
ATOM	4926	O	HOH	W	38	56.836	-25.915	35.276	1.00	54.31	O
ATOM	4927	O	HOH	W	39	53.914	24.322	19.731	1.00	41.25	O
ATOM	4928	O	HOH	W	40	28.860	-2.107	-3.273	1.00	16.41	O
ATOM	4929	O	HOH	W	41	44.164	3.010	44.987	1.00	29.00	O
ATOM	4930	O	HOH	W	42	44.791	32.626	21.307	1.00	49.96	O
ATOM	4931	O	HOH	W	43	39.715	-13.376	35.458	1.00	24.96	O
ATOM	4932	O	HOH	W	44	25.921	8.621	9.329	1.00	26.56	O
ATOM	4933	O	HOH	W	45	38.753	4.312	49.005	1.00	51.97	O
ATOM	4934	O	HOH	W	46	58.903	5.740	7.791	1.00	27.54	O
ATOM	4935	O	HOH	W	47	27.226	-11.395	12.963	1.00	25.89	O
ATOM	4936	O	HOH	W	48	40.091	4.314	36.727	1.00	46.51	O
ATOM	4937	O	HOH	W	49	48.515	7.616	30.861	1.00	43.74	O
ATOM	4938	O	HOH	W	50	28.718	-27.986	29.005	1.00	63.42	O
ATOM	4939	O	HOH	W	51	32.361	-11.238	8.172	1.00	37.80	O
ATOM	4940	O	HOH	W	52	33.363	-10.334	5.514	1.00	37.18	O
ATOM	4941	O	HOH	W	53	18.180	2.136	28.174	1.00	57.26	O
ATOM	4942	O	HOH	W	54	67.280	-11.392	8.706	1.00	29.55	O
ATOM	4943	O	HOH	W	55	71.544	1.658	14.206	1.00	59.28	O
ATOM	4944	O	HOH	W	56	26.449	10.114	6.226	1.00	70.68	O
ATOM	4945	O	HOH	W	57	54.453	-1.012	45.318	1.00	61.23	O
ATOM	4946	O	HOH	W	58	69.895	-3.128	23.527	1.00	53.56	O
ATOM	4947	O	HOH	W	59	20.903	-0.967	18.852	1.00	36.60	O
ATOM	4948	O	HOH	W	60	19.130	20.650	2.410	1.00	32.68	O

289/396

Figure 3A-89

ATOM	4949	O	HOH W	61	6.996	-2.746	16.016	1.00	46.59	O
ATOM	4950	O	HOH W	62	44.034	-20.682	31.215	1.00	47.72	O
ATOM	4951	O	HOH W	63	71.013	22.540	21.914	1.00	46.01	O
ATOM	4952	O	HOH W	64	40.799	-22.395	19.144	1.00	44.32	O
ATOM	4953	O	HOH W	65	47.443	3.173	39.454	1.00	59.18	O
ATOM	4954	O	HOH W	66	36.541	16.479	45.756	1.00	43.31	O
ATOM	4955	O	HOH W	67	31.548	-5.809	26.117	1.00	59.55	O
ATOM	4956	O	HOH W	68	38.570	1.275	7.030	1.00	57.22	O
ATOM	4957	O	HOH W	69	18.771	0.881	17.044	1.00	50.21	O
ATOM	4958	O	HOH W	70	38.858	-15.687	46.066	1.00	48.51	O
ATOM	4959	O	HOH W	71	42.791	-0.780	28.870	1.00	49.66	O
ATOM	4960	O	HOH W	72	61.464	-4.089	5.342	1.00	32.55	O
ATOM	4961	O	HOH W	73	63.496	-19.674	31.471	1.00	58.23	O
ATOM	4962	O	HOH W	74	39.067	-19.831	17.300	1.00	55.70	O
ATOM	4963	O	HOH W	75	41.098	27.379	10.240	1.00	77.20	O
ATOM	4964	O	HOH W	76	56.225	25.012	10.351	1.00	49.04	O

290/396

Figure 3B-1

	<u>Atom</u>	<u>Type</u>	<u>Resid</u>	<u>#</u>	<u>X</u>	<u>Y</u>	<u>Z</u>	<u>Occ</u>	<u>B</u>	
ATOM	1	CB	SER A	19	4.348	21.402	1.856	1.00	130.55	C
ATOM	2	OG	SER A	19	3.905	22.748	1.943	1.00	130.08	O
ATOM	3	C	SER A	19	3.942	19.134	0.874	1.00	129.08	C
ATOM	4	O	SER A	19	3.401	18.165	1.413	1.00	129.01	O
ATOM	5	N	SER A	19	2.039	20.499	1.715	1.00	130.27	N
ATOM	6	CA	SER A	19	3.371	20.541	1.042	1.00	130.01	C
ATOM	7	N	THR A	20	5.036	19.032	0.122	1.00	127.34	N
ATOM	8	CA	THR A	20	5.689	17.750	-0.122	1.00	125.41	C
ATOM	9	CB	THR A	20	7.127	17.949	-0.645	1.00	124.25	C
ATOM	10	OG1	THR A	20	7.131	18.940	-1.677	1.00	123.66	O
ATOM	11	CG2	THR A	20	7.671	16.649	-1.209	1.00	122.63	C
ATOM	12	C	THR A	20	5.760	16.938	1.169	1.00	125.00	C
ATOM	13	O	THR A	20	5.615	17.480	2.263	1.00	124.38	O
ATOM	14	N	ILE A	21	5.971	15.635	1.036	1.00	125.07	N
ATOM	15	CA	ILE A	21	6.083	14.762	2.199	1.00	125.00	C
ATOM	16	CB	ILE A	21	5.708	13.304	1.846	1.00	125.66	C
ATOM	17	CG2	ILE A	21	6.274	12.350	2.887	1.00	126.36	C
ATOM	18	CG1	ILE A	21	4.183	13.163	1.766	1.00	125.25	C
ATOM	19	CD1	ILE A	21	3.506	14.153	0.838	1.00	122.59	C
ATOM	20	C	ILE A	21	7.526	14.834	2.683	1.00	123.75	C
ATOM	21	O	ILE A	21	7.834	14.499	3.827	1.00	123.48	O
ATOM	22	N	GLU A	22	8.406	15.282	1.793	1.00	122.51	N
ATOM	23	CA	GLU A	22	9.813	15.452	2.118	1.00	122.03	C
ATOM	24	CB	GLU A	22	10.666	15.484	0.849	1.00	122.24	C
ATOM	25	CG	GLU A	22	12.158	15.695	1.085	1.00	120.83	C
ATOM	26	CD	GLU A	22	12.900	16.034	-0.195	1.00	121.12	C
ATOM	27	OE1	GLU A	22	12.766	15.264	-1.164	1.00	121.35	O
ATOM	28	OE2	GLU A	22	13.611	17.063	-0.238	1.00	120.12	O
ATOM	29	C	GLU A	22	9.876	16.805	2.806	1.00	122.68	C
ATOM	30	O	GLU A	22	10.775	17.605	2.567	1.00	123.54	O
ATOM	31	N	GLU A	23	8.881	17.069	3.638	1.00	122.56	N
ATOM	32	CA	GLU A	23	8.819	18.312	4.380	1.00	122.30	C
ATOM	33	CB	GLU A	23	8.027	19.366	3.613	1.00	122.69	C
ATOM	34	CG	GLU A	23	7.772	20.594	4.451	1.00	124.26	C
ATOM	35	CD	GLU A	23	9.038	21.079	5.116	1.00	125.00	C
ATOM	36	OE1	GLU A	23	8.945	21.775	6.155	1.00	125.16	O
ATOM	37	OE2	GLU A	23	10.127	20.763	4.589	1.00	124.76	O
ATOM	38	C	GLU A	23	8.160	18.044	5.720	1.00	122.82	C
ATOM	39	O	GLU A	23	8.451	18.713	6.712	1.00	122.71	O
ATOM	40	N	GLN A	24	7.263	17.061	5.741	1.00	123.26	N
ATOM	41	CA	GLN A	24	6.577	16.685	6.971	1.00	123.59	C
ATOM	42	CB	GLN A	24	5.566	15.565	6.707	1.00	124.54	C
ATOM	43	CG	GLN A	24	4.460	15.909	5.725	1.00	125.95	C
ATOM	44	CD	GLN A	24	3.506	14.749	5.503	1.00	126.83	C
ATOM	45	OE1	GLN A	24	2.851	14.280	6.437	1.00	126.80	O
ATOM	46	NE2	GLN A	24	3.427	14.276	4.264	1.00	126.28	N
ATOM	47	C	GLN A	24	7.661	16.173	7.908	1.00	122.72	C
ATOM	48	O	GLN A	24	7.465	16.066	9.117	1.00	122.73	O
ATOM	49	N	ALA A	25	8.809	15.854	7.321	1.00	120.84	N
ATOM	50	CA	ALA A	25	9.948	15.344	8.062	1.00	117.51	C
ATOM	51	CB	ALA A	25	10.531	14.138	7.344	1.00	117.24	C
ATOM	52	C	ALA A	25	11.009	16.422	8.207	1.00	115.72	C
ATOM	53	O	ALA A	25	11.631	16.550	9.258	1.00	115.70	O
ATOM	54	N	LYS A	26	11.225	17.201	7.155	1.00	113.15	N

291/396

Figure 3B-2

ATOM	55	CA	LYS	A	26	12.232	18.245	7.229	1.00	111.74	C
ATOM	56	CB	LYS	A	26	12.240	19.056	5.950	1.00	111.72	C
ATOM	57	CG	LYS	A	26	12.743	18.258	4.782	1.00	113.02	C
ATOM	58	CD	LYS	A	26	12.919	19.146	3.586	1.00	114.58	C
ATOM	59	CE	LYS	A	26	13.658	18.432	2.478	1.00	116.22	C
ATOM	60	NZ	LYS	A	26	13.782	19.254	1.241	1.00	118.58	N
ATOM	61	C	LYS	A	26	12.009	19.136	8.435	1.00	111.44	C
ATOM	62	O	LYS	A	26	12.849	19.967	8.780	1.00	111.58	O
ATOM	63	N	THR	A	27	10.859	18.946	9.069	1.00	111.34	N
ATOM	64	CA	THR	A	27	10.500	19.670	10.275	1.00	110.87	C
ATOM	65	CB	THR	A	27	9.077	20.237	10.220	1.00	111.75	C
ATOM	66	OG1	THR	A	27	8.652	20.551	11.554	1.00	110.15	O
ATOM	67	CG2	THR	A	27	8.110	19.229	9.593	1.00	111.18	C
ATOM	68	C	THR	A	27	10.549	18.665	11.412	1.00	110.31	C
ATOM	69	O	THR	A	27	11.242	18.876	12.405	1.00	111.22	O
ATOM	70	N	PHE	A	28	9.804	17.572	11.250	1.00	108.28	N
ATOM	71	CA	PHE	A	28	9.749	16.498	12.238	1.00	105.31	C
ATOM	72	CB	PHE	A	28	9.231	15.218	11.587	1.00	102.67	C
ATOM	73	CG	PHE	A	28	9.446	14.002	12.416	1.00	98.78	C
ATOM	74	CD1	PHE	A	28	9.005	13.960	13.720	1.00	99.15	C
ATOM	75	CD2	PHE	A	28	10.108	12.912	11.900	1.00	97.70	C
ATOM	76	CE1	PHE	A	28	9.221	12.855	14.493	1.00	100.31	C
ATOM	77	CE2	PHE	A	28	10.326	11.805	12.666	1.00	98.00	C
ATOM	78	CZ	PHE	A	28	9.882	11.776	13.968	1.00	99.61	C
ATOM	79	C	PHE	A	28	11.131	16.244	12.829	1.00	104.89	C
ATOM	80	O	PHE	A	28	11.269	15.891	14.003	1.00	105.19	O
ATOM	81	N	LEU	A	29	12.149	16.419	11.994	1.00	103.02	N
ATOM	82	CA	LEU	A	29	13.530	16.241	12.407	1.00	100.57	C
ATOM	83	CB	LEU	A	29	14.436	16.112	11.183	1.00	97.50	C
ATOM	84	CG	LEU	A	29	14.470	14.744	10.507	1.00	93.99	C
ATOM	85	CD1	LEU	A	29	13.140	14.049	10.656	1.00	92.96	C
ATOM	86	CD2	LEU	A	29	14.840	14.921	9.046	1.00	94.41	C
ATOM	87	C	LEU	A	29	13.952	17.447	13.228	1.00	99.96	C
ATOM	88	O	LEU	A	29	14.407	17.305	14.361	1.00	100.48	O
ATOM	89	N	ASP	A	30	13.789	18.635	12.650	1.00	98.15	N
ATOM	90	CA	ASP	A	30	14.165	19.869	13.327	1.00	96.43	C
ATOM	91	CB	ASP	A	30	13.949	21.065	12.408	1.00	99.30	C
ATOM	92	CG	ASP	A	30	14.396	22.364	13.042	1.00	102.92	C
ATOM	93	OD1	ASP	A	30	15.602	22.488	13.348	1.00	105.17	O
ATOM	94	OD2	ASP	A	30	13.547	23.260	13.243	1.00	105.96	O
ATOM	95	C	ASP	A	30	13.397	20.084	14.626	1.00	93.39	C
ATOM	96	O	ASP	A	30	13.912	20.673	15.571	1.00	92.26	O
ATOM	97	N	LYS	A	31	12.159	19.613	14.668	1.00	91.02	N
ATOM	98	CA	LYS	A	31	11.345	19.751	15.866	1.00	89.77	C
ATOM	99	CB	LYS	A	31	9.870	19.470	15.532	1.00	89.05	C
ATOM	100	CG	LYS	A	31	8.856	20.370	16.241	1.00	86.48	C
ATOM	101	CD	LYS	A	31	8.288	19.744	17.503	1.00	82.32	C
ATOM	102	CE	LYS	A	31	7.299	18.658	17.174	1.00	77.90	C
ATOM	103	NZ	LYS	A	31	6.709	18.079	18.410	1.00	79.27	N
ATOM	104	C	LYS	A	31	11.888	18.713	16.845	1.00	88.84	C
ATOM	105	O	LYS	A	31	11.570	18.723	18.030	1.00	89.69	O
ATOM	106	N	PHE	A	32	12.721	17.818	16.324	1.00	87.12	N
ATOM	107	CA	PHE	A	32	13.337	16.758	17.111	1.00	84.54	C
ATOM	108	CB	PHE	A	32	13.503	15.513	16.229	1.00	86.94	C
ATOM	109	CG	PHE	A	32	14.355	14.434	16.835	1.00	90.28	C
ATOM	110	CD1	PHE	A	32	15.734	14.459	16.698	1.00	90.70	C

292/396

Figure 3B-3

ATOM	111	CD2	PHE	A	32	13.776	13.393	17.546	1.00	90.93	C
ATOM	112	CE1	PHE	A	32	16.519	13.466	17.259	1.00	90.14	C
ATOM	113	CE2	PHE	A	32	14.558	12.397	18.110	1.00	91.13	C
ATOM	114	CZ	PHE	A	32	15.929	12.433	17.966	1.00	89.68	C
ATOM	115	C	PHE	A	32	14.686	17.233	17.654	1.00	81.10	C
ATOM	116	O	PHE	A	32	14.939	17.185	18.855	1.00	81.10	O
ATOM	117	N	ASN	A	33	15.541	17.706	16.759	1.00	76.75	N
ATOM	118	CA	ASN	A	33	16.861	18.200	17.127	1.00	75.68	C
ATOM	119	CB	ASN	A	33	17.508	18.866	15.921	1.00	75.19	C
ATOM	120	CG	ASN	A	33	17.604	17.945	14.744	1.00	78.18	C
ATOM	121	OD1	ASN	A	33	18.046	18.343	13.669	1.00	80.31	O
ATOM	122	ND2	ASN	A	33	17.190	16.697	14.936	1.00	78.84	N
ATOM	123	C	ASN	A	33	16.868	19.202	18.280	1.00	75.29	C
ATOM	124	O	ASN	A	33	17.901	19.435	18.910	1.00	76.41	O
ATOM	125	N	HIS	A	34	15.723	19.801	18.560	1.00	72.30	N
ATOM	126	CA	HIS	A	34	15.670	20.797	19.606	1.00	67.12	C
ATOM	127	CB	HIS	A	34	14.799	21.949	19.153	1.00	64.92	C
ATOM	128	CG	HIS	A	34	15.464	22.813	18.140	1.00	59.27	C
ATOM	129	CD2	HIS	A	34	15.494	22.740	16.793	1.00	59.13	C
ATOM	130	ND1	HIS	A	34	16.294	23.853	18.490	1.00	61.34	N
ATOM	131	CE1	HIS	A	34	16.811	24.387	17.398	1.00	60.68	C
ATOM	132	NE2	HIS	A	34	16.342	23.728	16.355	1.00	62.80	N
ATOM	133	C	HIS	A	34	15.231	20.307	20.947	1.00	66.75	C
ATOM	134	O	HIS	A	34	15.663	20.847	21.956	1.00	65.36	O
ATOM	135	N	GLU	A	35	14.362	19.304	20.975	1.00	67.83	N
ATOM	136	CA	GLU	A	35	13.931	18.766	22.256	1.00	73.06	C
ATOM	137	CB	GLU	A	35	12.566	18.073	22.148	1.00	71.44	C
ATOM	138	CG	GLU	A	35	12.236	17.238	23.391	1.00	74.91	C
ATOM	139	CD	GLU	A	35	10.748	17.092	23.660	1.00	75.34	C
ATOM	140	OE1	GLU	A	35	9.982	16.939	22.686	1.00	78.40	O
ATOM	141	OE2	GLU	A	35	10.351	17.112	24.848	1.00	72.34	O
ATOM	142	C	GLU	A	35	14.996	17.773	22.732	1.00	76.67	C
ATOM	143	O	GLU	A	35	15.365	17.742	23.920	1.00	75.64	O
ATOM	144	N	ALA	A	36	15.499	16.978	21.789	1.00	78.36	N
ATOM	145	CA	ALA	A	36	16.529	15.992	22.076	1.00	79.23	C
ATOM	146	CB	ALA	A	36	16.967	15.322	20.790	1.00	79.67	C
ATOM	147	C	ALA	A	36	17.729	16.649	22.772	1.00	79.98	C
ATOM	148	O	ALA	A	36	18.053	16.317	23.911	1.00	80.87	O
ATOM	149	N	GLU	A	37	18.380	17.584	22.089	1.00	78.36	N
ATOM	150	CA	GLU	A	37	19.529	18.274	22.658	1.00	78.56	C
ATOM	151	CB	GLU	A	37	19.756	19.596	21.928	1.00	78.76	C
ATOM	152	CG	GLU	A	37	20.649	20.572	22.672	1.00	78.88	C
ATOM	153	CD	GLU	A	37	20.925	21.837	21.876	1.00	78.68	C
ATOM	154	OE1	GLU	A	37	21.661	21.751	20.866	1.00	75.76	O
ATOM	155	OE2	GLU	A	37	20.399	22.910	22.263	1.00	76.65	O
ATOM	156	C	GLU	A	37	19.370	18.535	24.152	1.00	79.51	C
ATOM	157	O	GLU	A	37	20.198	18.113	24.951	1.00	78.17	O
ATOM	158	N	ASP	A	38	18.301	19.228	24.529	1.00	82.55	N
ATOM	159	CA	ASP	A	38	18.053	19.535	25.937	1.00	84.86	C
ATOM	160	CB	ASP	A	38	16.876	20.510	26.083	1.00	90.48	C
ATOM	161	CG	ASP	A	38	16.320	20.549	27.506	1.00	95.34	C
ATOM	162	OD1	ASP	A	38	17.135	20.591	28.457	1.00	100.31	O
ATOM	163	OD2	ASP	A	38	15.075	20.545	27.676	1.00	94.74	O
ATOM	164	C	ASP	A	38	17.758	18.278	26.732	1.00	82.94	C
ATOM	165	O	ASP	A	38	18.262	18.107	27.844	1.00	80.92	O
ATOM	166	N	LEU	A	39	16.930	17.410	26.157	1.00	80.73	N

293/396

Figure 3B-4

ATOM	167	CA	LEU	A	39	16.555	16.162	26.807	1.00	79.45	C
ATOM	168	CB	LEU	A	39	15.522	15.416	25.959	1.00	79.45	C
ATOM	169	CG	LEU	A	39	14.389	14.743	26.739	1.00	78.44	C
ATOM	170	CD1	LEU	A	39	14.967	13.732	27.716	1.00	79.86	C
ATOM	171	CD2	LEU	A	39	13.584	15.803	27.484	1.00	78.44	C
ATOM	172	C	LEU	A	39	17.800	15.305	27.005	1.00	77.07	C
ATOM	173	O	LEU	A	39	17.922	14.590	27.998	1.00	79.46	O
ATOM	174	N	PHE	A	40	18.719	15.382	26.050	1.00	72.94	N
ATOM	175	CA	PHE	A	40	19.977	14.653	26.124	1.00	69.26	C
ATOM	176	CB	PHE	A	40	20.760	14.837	24.832	1.00	65.78	C
ATOM	177	CG	PHE	A	40	22.083	14.137	24.814	1.00	60.42	C
ATOM	178	CD1	PHE	A	40	22.166	12.784	25.045	1.00	58.70	C
ATOM	179	CD2	PHE	A	40	23.238	14.824	24.498	1.00	61.08	C
ATOM	180	CE1	PHE	A	40	23.369	12.130	24.956	1.00	56.04	C
ATOM	181	CE2	PHE	A	40	24.442	14.170	24.407	1.00	58.92	C
ATOM	182	CZ	PHE	A	40	24.504	12.821	24.635	1.00	55.71	C
ATOM	183	C	PHE	A	40	20.746	15.278	27.270	1.00	69.00	C
ATOM	184	O	PHE	A	40	20.945	14.658	28.308	1.00	68.88	O
ATOM	185	N	TYR	A	41	21.161	16.524	27.061	1.00	68.39	N
ATOM	186	CA	TYR	A	41	21.898	17.305	28.049	1.00	66.65	C
ATOM	187	CB	TYR	A	41	21.811	18.781	27.680	1.00	63.39	C
ATOM	188	CG	TYR	A	41	22.631	19.692	28.554	1.00	61.87	C
ATOM	189	CD1	TYR	A	41	23.827	20.229	28.094	1.00	60.24	C
ATOM	190	CE1	TYR	A	41	24.579	21.063	28.890	1.00	59.70	C
ATOM	191	CD2	TYR	A	41	22.213	20.017	29.842	1.00	58.62	C
ATOM	192	CE2	TYR	A	41	22.959	20.843	30.642	1.00	56.18	C
ATOM	193	CZ	TYR	A	41	24.142	21.364	30.163	1.00	58.81	C
ATOM	194	OH	TYR	A	41	24.905	22.178	30.962	1.00	60.24	O
ATOM	195	C	TYR	A	41	21.325	17.097	29.452	1.00	67.68	C
ATOM	196	O	TYR	A	41	22.025	17.210	30.451	1.00	64.91	O
ATOM	197	N	GLN	A	42	20.037	16.807	29.525	1.00	71.47	N
ATOM	198	CA	GLN	A	42	19.409	16.583	30.815	1.00	76.27	C
ATOM	199	CB	GLN	A	42	17.895	16.406	30.645	1.00	81.46	C
ATOM	200	CG	GLN	A	42	17.026	17.372	31.456	1.00	84.37	C
ATOM	201	CD	GLN	A	42	17.037	18.800	30.920	1.00	87.16	C
ATOM	202	OE1	GLN	A	42	16.002	19.475	30.917	1.00	88.17	O
ATOM	203	NE2	GLN	A	42	18.205	19.271	30.477	1.00	85.87	N
ATOM	204	C	GLN	A	42	20.026	15.314	31.383	1.00	75.97	C
ATOM	205	O	GLN	A	42	20.338	15.238	32.570	1.00	76.83	O
ATOM	206	N	SER	A	43	20.197	14.321	30.514	1.00	75.24	N
ATOM	207	CA	SER	A	43	20.787	13.038	30.883	1.00	74.33	C
ATOM	208	CB	SER	A	43	20.426	11.981	29.830	1.00	73.02	C
ATOM	209	OG	SER	A	43	20.550	10.668	30.348	1.00	70.66	O
ATOM	210	C	SER	A	43	22.316	13.201	30.987	1.00	73.82	C
ATOM	211	O	SER	A	43	22.894	12.974	32.048	1.00	74.33	O
ATOM	212	N	SER	A	44	22.962	13.612	29.896	1.00	71.85	N
ATOM	213	CA	SER	A	44	24.411	13.820	29.888	1.00	70.11	C
ATOM	214	CB	SER	A	44	24.830	14.655	28.672	1.00	68.66	C
ATOM	215	OG	SER	A	44	24.557	13.983	27.459	1.00	69.99	O
ATOM	216	C	SER	A	44	24.902	14.520	31.160	1.00	70.39	C
ATOM	217	O	SER	A	44	26.029	14.303	31.599	1.00	72.57	O
ATOM	218	N	LEU	A	45	24.057	15.361	31.747	1.00	69.24	N
ATOM	219	CA	LEU	A	45	24.425	16.081	32.957	1.00	66.54	C
ATOM	220	CB	LEU	A	45	23.549	17.322	33.142	1.00	70.99	C
ATOM	221	CG	LEU	A	45	24.220	18.696	33.027	1.00	74.26	C
ATOM	222	CD1	LEU	A	45	23.283	19.761	33.605	1.00	71.34	C

294/396

Figure 3B-5

ATOM	223	CD2	LEU	A	45	25.559	18.690	33.779	1.00	74.55	C
ATOM	224	C	LEU	A	45	24.284	15.201	34.176	1.00	64.06	C
ATOM	225	O	LEU	A	45	25.182	15.144	34.998	1.00	66.31	O
ATOM	226	N	ALA	A	46	23.147	14.529	34.301	1.00	59.74	N
ATOM	227	CA	ALA	A	46	22.914	13.656	35.438	1.00	57.80	C
ATOM	228	CB	ALA	A	46	21.516	13.126	35.398	1.00	58.19	C
ATOM	229	C	ALA	A	46	23.893	12.511	35.346	1.00	59.30	C
ATOM	230	O	ALA	A	46	24.473	12.085	36.340	1.00	60.83	O
ATOM	231	N	SER	A	47	24.064	12.026	34.124	1.00	60.60	N
ATOM	232	CA	SER	A	47	24.960	10.929	33.811	1.00	60.02	C
ATOM	233	CB	SER	A	47	24.881	10.624	32.319	1.00	60.44	C
ATOM	234	OG	SER	A	47	25.735	9.562	31.959	1.00	65.45	O
ATOM	235	C	SER	A	47	26.376	11.316	34.183	1.00	61.69	C
ATOM	236	O	SER	A	47	27.208	10.463	34.474	1.00	66.37	O
ATOM	237	N	TRP	A	48	26.655	12.611	34.173	1.00	60.14	N
ATOM	238	CA	TRP	A	48	27.980	13.083	34.523	1.00	59.06	C
ATOM	239	CB	TRP	A	48	28.196	14.475	33.944	1.00	55.77	C
ATOM	240	CG	TRP	A	48	29.332	15.229	34.533	1.00	52.02	C
ATOM	241	CD2	TRP	A	48	30.637	15.389	33.974	1.00	47.79	C
ATOM	242	CE2	TRP	A	48	31.345	16.267	34.812	1.00	47.77	C
ATOM	243	CE3	TRP	A	48	31.271	14.882	32.849	1.00	45.31	C
ATOM	244	CD1	TRP	A	48	29.306	15.981	35.665	1.00	52.27	C
ATOM	245	NE1	TRP	A	48	30.510	16.614	35.837	1.00	52.54	N
ATOM	246	CZ2	TRP	A	48	32.652	16.649	34.558	1.00	45.47	C
ATOM	247	CZ3	TRP	A	48	32.568	15.262	32.598	1.00	50.46	C
ATOM	248	CH2	TRP	A	48	33.247	16.140	33.447	1.00	47.98	C
ATOM	249	C	TRP	A	48	28.193	13.083	36.028	1.00	60.72	C
ATOM	250	O	TRP	A	48	29.257	12.703	36.503	1.00	61.49	O
ATOM	251	N	ASN	A	49	27.181	13.495	36.781	1.00	63.23	N
ATOM	252	CA	ASN	A	49	27.304	13.512	38.233	1.00	68.47	C
ATOM	253	CB	ASN	A	49	26.001	13.982	38.885	1.00	71.63	C
ATOM	254	CG	ASN	A	49	25.837	15.497	38.843	1.00	77.54	C
ATOM	255	OD1	ASN	A	49	24.873	16.039	39.386	1.00	81.48	O
ATOM	256	ND2	ASN	A	49	26.780	16.187	38.198	1.00	78.02	N
ATOM	257	C	ASN	A	49	27.668	12.125	38.739	1.00	69.24	C
ATOM	258	O	ASN	A	49	28.398	11.979	39.721	1.00	66.14	O
ATOM	259	N	TYR	A	50	27.160	11.106	38.055	1.00	71.87	N
ATOM	260	CA	TYR	A	50	27.446	9.727	38.429	1.00	73.01	C
ATOM	261	CB	TYR	A	50	26.646	8.748	37.579	1.00	71.50	C
ATOM	262	CG	TYR	A	50	27.045	7.314	37.825	1.00	72.54	C
ATOM	263	CD1	TYR	A	50	26.579	6.628	38.932	1.00	74.91	C
ATOM	264	CE1	TYR	A	50	26.921	5.309	39.155	1.00	78.08	C
ATOM	265	CD2	TYR	A	50	27.877	6.643	36.945	1.00	71.77	C
ATOM	266	CE2	TYR	A	50	28.228	5.327	37.157	1.00	75.39	C
ATOM	267	CZ	TYR	A	50	27.744	4.657	38.265	1.00	78.77	C
ATOM	268	OH	TYR	A	50	28.069	3.329	38.484	1.00	80.73	O
ATOM	269	C	TYR	A	50	28.919	9.421	38.227	1.00	72.15	C
ATOM	270	O	TYR	A	50	29.616	9.018	39.152	1.00	73.56	O
ATOM	271	N	ASN	A	51	29.386	9.608	37.001	1.00	69.91	N
ATOM	272	CA	ASN	A	51	30.771	9.326	36.690	1.00	68.73	C
ATOM	273	CB	ASN	A	51	31.006	9.433	35.186	1.00	65.89	C
ATOM	274	CG	ASN	A	51	30.337	8.328	34.428	1.00	63.79	C
ATOM	275	OD1	ASN	A	51	29.128	8.163	34.502	1.00	62.56	O
ATOM	276	ND2	ASN	A	51	31.121	7.550	33.698	1.00	68.16	N
ATOM	277	C	ASN	A	51	31.738	10.222	37.428	1.00	68.22	C
ATOM	278	O	ASN	A	51	32.944	10.110	37.244	1.00	68.71	O

295/396

Figure 3B-6

ATOM	279	N	THR	A	52	31.224	11.115	38.261	1.00	67.86	N
ATOM	280	CA	THR	A	52	32.116	11.993	39.000	1.00	71.26	C
ATOM	281	CB	THR	A	52	31.947	13.465	38.580	1.00	72.62	C
ATOM	282	OG1	THR	A	52	32.110	13.587	37.162	1.00	73.77	O
ATOM	283	CG2	THR	A	52	33.000	14.319	39.249	1.00	73.72	C
ATOM	284	C	THR	A	52	31.886	11.866	40.499	1.00	72.17	C
ATOM	285	O	THR	A	52	32.495	12.575	41.294	1.00	72.46	O
ATOM	286	N	ASN	A	53	31.006	10.948	40.877	1.00	73.19	N
ATOM	287	CA	ASN	A	53	30.688	10.706	42.277	1.00	75.21	C
ATOM	288	CB	ASN	A	53	30.039	11.939	42.905	1.00	77.80	C
ATOM	289	CG	ASN	A	53	29.795	11.775	44.393	1.00	78.41	C
ATOM	290	OD1	ASN	A	53	29.197	12.644	45.033	1.00	79.54	O
ATOM	291	ND2	ASN	A	53	30.264	10.659	44.955	1.00	77.92	N
ATOM	292	C	ASN	A	53	29.709	9.557	42.306	1.00	76.66	C
ATOM	293	O	ASN	A	53	28.506	9.759	42.174	1.00	75.49	O
ATOM	294	N	ILE	A	54	30.222	8.349	42.477	1.00	80.29	N
ATOM	295	CA	ILE	A	54	29.357	7.190	42.487	1.00	85.62	C
ATOM	296	CB	ILE	A	54	30.155	5.902	42.168	1.00	85.71	C
ATOM	297	CG2	ILE	A	54	29.196	4.745	41.873	1.00	85.33	C
ATOM	298	CG1	ILE	A	54	31.037	6.139	40.938	1.00	82.71	C
ATOM	299	CD1	ILE	A	54	31.719	4.905	40.426	1.00	82.16	C
ATOM	300	C	ILE	A	54	28.617	7.056	43.812	1.00	89.76	C
ATOM	301	O	ILE	A	54	28.682	6.028	44.484	1.00	91.52	O
ATOM	302	N	THR	A	55	27.919	8.125	44.183	1.00	94.66	N
ATOM	303	CA	THR	A	55	27.124	8.142	45.404	1.00	98.10	C
ATOM	304	CB	THR	A	55	26.391	9.499	45.587	1.00	97.74	C
ATOM	305	OG1	THR	A	55	27.339	10.567	45.534	1.00	99.50	O
ATOM	306	CG2	THR	A	55	25.658	9.549	46.928	1.00	97.84	C
ATOM	307	C	THR	A	55	26.064	7.069	45.200	1.00	100.76	C
ATOM	308	O	THR	A	55	26.311	5.873	45.373	1.00	100.98	O
ATOM	309	N	GLU	A	56	24.883	7.524	44.808	1.00	102.73	N
ATOM	310	CA	GLU	A	56	23.754	6.654	44.555	1.00	105.02	C
ATOM	311	CB	GLU	A	56	23.395	5.857	45.801	1.00	104.94	C
ATOM	312	CG	GLU	A	56	22.801	4.508	45.473	1.00	106.38	C
ATOM	313	CD	GLU	A	56	21.887	4.566	44.267	1.00	106.66	C
ATOM	314	OE1	GLU	A	56	20.960	5.402	44.269	1.00	108.39	O
ATOM	315	OE2	GLU	A	56	22.094	3.776	43.320	1.00	106.28	O
ATOM	316	C	GLU	A	56	22.621	7.588	44.190	1.00	106.52	C
ATOM	317	O	GLU	A	56	21.883	7.347	43.240	1.00	107.27	O
ATOM	318	N	GLU	A	57	22.483	8.663	44.957	1.00	108.04	N
ATOM	319	CA	GLU	A	57	21.459	9.649	44.663	1.00	109.96	C
ATOM	320	CB	GLU	A	57	21.666	10.906	45.504	1.00	111.98	C
ATOM	321	CG	GLU	A	57	22.119	10.606	46.902	1.00	116.66	C
ATOM	322	CD	GLU	A	57	21.292	9.514	47.528	1.00	119.50	C
ATOM	323	OE1	GLU	A	57	20.100	9.758	47.817	1.00	119.76	O
ATOM	324	OE2	GLU	A	57	21.837	8.406	47.716	1.00	122.76	O
ATOM	325	C	GLU	A	57	21.723	9.982	43.207	1.00	109.41	C
ATOM	326	O	GLU	A	57	20.807	10.095	42.398	1.00	109.94	O
ATOM	327	N	ASN	A	58	23.007	10.113	42.891	1.00	107.83	N
ATOM	328	CA	ASN	A	58	23.454	10.430	41.551	1.00	105.68	C
ATOM	329	CB	ASN	A	58	24.957	10.676	41.566	1.00	107.29	C
ATOM	330	CG	ASN	A	58	25.351	11.765	42.540	1.00	109.12	C
ATOM	331	OD1	ASN	A	58	25.034	11.696	43.728	1.00	110.89	O
ATOM	332	ND2	ASN	A	58	26.043	12.780	42.041	1.00	111.06	N
ATOM	333	C	ASN	A	58	23.110	9.299	40.597	1.00	104.06	C
ATOM	334	O	ASN	A	58	22.787	9.542	39.435	1.00	104.13	O

296/396

Figure 3B-7

ATOM	335	N	VAL	A	59	23.179	8.066	41.087	1.00	101.54	N
ATOM	336	CA	VAL	A	59	22.850	6.910	40.261	1.00	101.07	C
ATOM	337	CB	VAL	A	59	22.920	5.600	41.054	1.00	100.82	C
ATOM	338	CG1	VAL	A	59	22.067	4.536	40.374	1.00	98.55	C
ATOM	339	CG2	VAL	A	59	24.358	5.137	41.157	1.00	101.83	C
ATOM	340	C	VAL	A	59	21.435	7.043	39.722	1.00	102.05	C
ATOM	341	O	VAL	A	59	21.229	7.120	38.509	1.00	103.90	O
ATOM	342	N	GLN	A	60	20.465	7.069	40.634	1.00	100.76	N
ATOM	343	CA	GLN	A	60	19.059	7.193	40.271	1.00	98.03	C
ATOM	344	CB	GLN	A	60	18.196	7.271	41.531	1.00	99.92	C
ATOM	345	CG	GLN	A	60	18.242	6.010	42.367	1.00	101.47	C
ATOM	346	CD	GLN	A	60	17.782	4.795	41.588	1.00	103.67	C
ATOM	347	OE1	GLN	A	60	16.584	4.602	41.364	1.00	104.28	O
ATOM	348	NE2	GLN	A	60	18.735	3.974	41.155	1.00	104.30	N
ATOM	349	C	GLN	A	60	18.811	8.411	39.393	1.00	95.50	C
ATOM	350	O	GLN	A	60	18.245	8.289	38.309	1.00	95.44	O
ATOM	351	N	ASN	A	61	19.236	9.580	39.858	1.00	93.11	N
ATOM	352	CA	ASN	A	61	19.065	10.806	39.091	1.00	93.15	C
ATOM	353	CB	ASN	A	61	19.998	11.904	39.605	1.00	95.86	C
ATOM	354	CG	ASN	A	61	19.723	12.287	41.042	1.00	98.05	C
ATOM	355	OD1	ASN	A	61	20.373	13.180	41.594	1.00	98.14	O
ATOM	356	ND2	ASN	A	61	18.757	11.614	41.660	1.00	98.92	N
ATOM	357	C	ASN	A	61	19.412	10.528	37.636	1.00	92.44	C
ATOM	358	O	ASN	A	61	18.740	11.002	36.719	1.00	91.59	O
ATOM	359	N	MET	A	62	20.477	9.753	37.446	1.00	90.67	N
ATOM	360	CA	MET	A	62	20.958	9.398	36.123	1.00	88.92	C
ATOM	361	CB	MET	A	62	22.349	8.773	36.218	1.00	87.50	C
ATOM	362	CG	MET	A	62	22.956	8.388	34.868	1.00	83.08	C
ATOM	363	SD	MET	A	62	24.462	7.401	35.015	1.00	73.36	S
ATOM	364	CE	MET	A	62	23.776	5.783	35.132	1.00	71.79	C
ATOM	365	C	MET	A	62	20.031	8.442	35.388	1.00	90.30	C
ATOM	366	O	MET	A	62	19.500	8.790	34.336	1.00	92.69	O
ATOM	367	N	ASN	A	63	19.827	7.239	35.922	1.00	89.96	N
ATOM	368	CA	ASN	A	63	18.964	6.288	35.228	1.00	89.83	C
ATOM	369	CB	ASN	A	63	19.213	4.846	35.712	1.00	93.16	C
ATOM	370	CG	ASN	A	63	18.831	4.634	37.151	1.00	95.80	C
ATOM	371	OD1	ASN	A	63	17.707	4.937	37.556	1.00	99.42	O
ATOM	372	ND2	ASN	A	63	19.760	4.096	37.937	1.00	94.72	N
ATOM	373	C	ASN	A	63	17.492	6.666	35.332	1.00	87.09	C
ATOM	374	O	ASN	A	63	16.602	5.819	35.321	1.00	85.29	O
ATOM	375	N	ASN	A	64	17.268	7.970	35.437	1.00	86.70	N
ATOM	376	CA	ASN	A	64	15.941	8.569	35.488	1.00	86.33	C
ATOM	377	CB	ASN	A	64	15.716	9.312	36.812	1.00	85.39	C
ATOM	378	CG	ASN	A	64	15.289	8.385	37.948	1.00	86.46	C
ATOM	379	OD1	ASN	A	64	15.801	7.270	38.084	1.00	86.46	O
ATOM	380	ND2	ASN	A	64	14.356	8.851	38.776	1.00	83.31	N
ATOM	381	C	ASN	A	64	15.961	9.555	34.326	1.00	86.16	C
ATOM	382	O	ASN	A	64	15.020	9.627	33.544	1.00	86.50	O
ATOM	383	N	ALA	A	65	17.063	10.290	34.208	1.00	86.26	N
ATOM	384	CA	ALA	A	65	17.246	11.268	33.141	1.00	87.83	C
ATOM	385	CB	ALA	A	65	18.528	12.061	33.376	1.00	86.85	C
ATOM	386	C	ALA	A	65	17.309	10.583	31.781	1.00	89.60	C
ATOM	387	O	ALA	A	65	16.864	11.135	30.769	1.00	90.71	O
ATOM	388	N	GLY	A	66	17.878	9.381	31.765	1.00	90.41	N
ATOM	389	CA	GLY	A	66	17.996	8.631	30.529	1.00	91.49	C
ATOM	390	C	GLY	A	66	16.818	7.698	30.325	1.00	92.87	C

297/396

Figure 3B-8

ATOM	391	O	GLY	A	66	16.489	7.344	29.194	1.00	92.76	O
ATOM	392	N	ASP	A	67	16.186	7.293	31.423	1.00	93.62	N
ATOM	393	CA	ASP	A	67	15.036	6.407	31.351	1.00	93.84	C
ATOM	394	CB	ASP	A	67	14.626	5.971	32.753	1.00	95.10	C
ATOM	395	CG	ASP	A	67	13.783	4.714	32.747	1.00	98.64	C
ATOM	396	OD1	ASP	A	67	12.885	4.602	31.880	1.00	98.89	O
ATOM	397	OD2	ASP	A	67	14.014	3.843	33.617	1.00	100.20	O
ATOM	398	C	ASP	A	67	13.902	7.186	30.689	1.00	94.29	C
ATOM	399	O	ASP	A	67	13.036	6.612	30.026	1.00	95.50	O
ATOM	400	N	LYS	A	68	13.919	8.503	30.884	1.00	94.03	N
ATOM	401	CA	LYS	A	68	12.927	9.401	30.301	1.00	92.16	C
ATOM	402	CB	LYS	A	68	12.898	10.733	31.046	1.00	95.54	C
ATOM	403	CG	LYS	A	68	12.479	11.911	30.174	1.00	100.89	C
ATOM	404	CD	LYS	A	68	11.068	11.741	29.586	1.00	107.99	C
ATOM	405	CE	LYS	A	68	9.950	11.957	30.620	1.00	108.88	C
ATOM	406	NZ	LYS	A	68	9.807	13.384	31.048	1.00	109.23	N
ATOM	407	C	LYS	A	68	13.316	9.656	28.863	1.00	89.33	C
ATOM	408	O	LYS	A	68	12.464	9.733	27.982	1.00	88.57	O
ATOM	409	N	TRP	A	69	14.615	9.815	28.639	1.00	87.60	N
ATOM	410	CA	TRP	A	69	15.127	10.038	27.298	1.00	87.02	C
ATOM	411	CB	TRP	A	69	16.626	10.344	27.342	1.00	84.45	C
ATOM	412	CG	TRP	A	69	17.299	10.149	26.027	1.00	83.21	C
ATOM	413	CD2	TRP	A	69	17.650	11.164	25.082	1.00	83.60	C
ATOM	414	CE2	TRP	A	69	18.205	10.517	23.963	1.00	82.34	C
ATOM	415	CE3	TRP	A	69	17.548	12.557	25.071	1.00	83.92	C
ATOM	416	CD1	TRP	A	69	17.650	8.964	25.461	1.00	82.77	C
ATOM	417	NE1	TRP	A	69	18.192	9.173	24.221	1.00	83.29	N
ATOM	418	CZ2	TRP	A	69	18.654	11.210	22.845	1.00	81.37	C
ATOM	419	CZ3	TRP	A	69	17.996	13.244	23.959	1.00	83.20	C
ATOM	420	CH2	TRP	A	69	18.542	12.570	22.862	1.00	81.98	C
ATOM	421	C	TRP	A	69	14.865	8.752	26.533	1.00	86.82	C
ATOM	422	O	TRP	A	69	14.618	8.756	25.329	1.00	86.03	O
ATOM	423	N	SER	A	70	14.923	7.645	27.262	1.00	87.94	N
ATOM	424	CA	SER	A	70	14.673	6.328	26.697	1.00	88.37	C
ATOM	425	CB	SER	A	70	14.778	5.272	27.810	1.00	89.52	C
ATOM	426	OG	SER	A	70	14.687	3.947	27.317	1.00	90.63	O
ATOM	427	C	SER	A	70	13.250	6.403	26.148	1.00	87.10	C
ATOM	428	O	SER	A	70	13.004	6.151	24.966	1.00	84.69	O
ATOM	429	N	ALA	A	71	12.328	6.784	27.029	1.00	87.04	N
ATOM	430	CA	ALA	A	71	10.916	6.926	26.699	1.00	86.10	C
ATOM	431	CB	ALA	A	71	10.136	7.321	27.955	1.00	84.95	C
ATOM	432	C	ALA	A	71	10.700	7.960	25.585	1.00	85.41	C
ATOM	433	O	ALA	A	71	9.839	7.788	24.724	1.00	85.63	O
ATOM	434	N	PHE	A	72	11.478	9.035	25.604	1.00	84.07	N
ATOM	435	CA	PHE	A	72	11.367	10.062	24.578	1.00	82.95	C
ATOM	436	CB	PHE	A	72	12.323	11.211	24.878	1.00	81.31	C
ATOM	437	CG	PHE	A	72	12.672	12.036	23.670	1.00	80.61	C
ATOM	438	CD1	PHE	A	72	11.693	12.709	22.965	1.00	78.33	C
ATOM	439	CD2	PHE	A	72	13.986	12.143	23.243	1.00	81.96	C
ATOM	440	CE1	PHE	A	72	12.016	13.475	21.863	1.00	78.73	C
ATOM	441	CE2	PHE	A	72	14.315	12.911	22.135	1.00	80.96	C
ATOM	442	CZ	PHE	A	72	13.328	13.577	21.447	1.00	79.56	C
ATOM	443	C	PHE	A	72	11.706	9.499	23.205	1.00	83.80	C
ATOM	444	O	PHE	A	72	10.903	9.548	22.279	1.00	83.65	O
ATOM	445	N	LEU	A	73	12.914	8.967	23.087	1.00	85.92	N
ATOM	446	CA	LEU	A	73	13.395	8.409	21.836	1.00	86.61	C

298/396

Figure 3B-9

ATOM	447	CB	LEU	A	73	14.833	7.929	22.009	1.00	86.02	C
ATOM	448	CG	LEU	A	73	15.774	8.341	20.879	1.00	86.21	C
ATOM	449	CD1	LEU	A	73	15.468	9.775	20.469	1.00	86.18	C
ATOM	450	CD2	LEU	A	73	17.221	8.190	21.328	1.00	85.09	C
ATOM	451	C	LEU	A	73	12.507	7.267	21.396	1.00	87.86	C
ATOM	452	O	LEU	A	73	12.208	7.123	20.216	1.00	87.77	O
ATOM	453	N	LYS	A	74	12.087	6.448	22.349	1.00	91.00	N
ATOM	454	CA	LYS	A	74	11.213	5.327	22.034	1.00	95.98	C
ATOM	455	CB	LYS	A	74	10.804	4.593	23.322	1.00	97.06	C
ATOM	456	CG	LYS	A	74	9.469	3.846	23.244	1.00	96.80	C
ATOM	457	CD	LYS	A	74	9.470	2.737	22.201	1.00	96.74	C
ATOM	458	CE	LYS	A	74	8.095	2.085	22.097	1.00	96.31	C
ATOM	459	NZ	LYS	A	74	7.615	1.537	23.404	1.00	94.63	N
ATOM	460	C	LYS	A	74	9.978	5.859	21.316	1.00	97.84	C
ATOM	461	O	LYS	A	74	9.744	5.555	20.144	1.00	98.67	O
ATOM	462	N	GLU	A	75	9.201	6.664	22.034	1.00	99.13	N
ATOM	463	CA	GLU	A	75	7.986	7.256	21.500	1.00	99.76	C
ATOM	464	CB	GLU	A	75	7.447	8.286	22.502	1.00	102.59	C
ATOM	465	CG	GLU	A	75	6.348	9.212	21.996	1.00	107.13	C
ATOM	466	CD	GLU	A	75	6.897	10.495	21.381	1.00	110.55	C
ATOM	467	OE1	GLU	A	75	7.391	10.458	20.233	1.00	111.36	O
ATOM	468	OE2	GLU	A	75	6.844	11.546	22.056	1.00	112.53	O
ATOM	469	C	GLU	A	75	8.239	7.890	20.137	1.00	99.06	C
ATOM	470	O	GLU	A	75	7.526	7.608	19.176	1.00	100.58	O
ATOM	471	N	GLN	A	76	9.262	8.730	20.041	1.00	97.18	N
ATOM	472	CA	GLN	A	76	9.564	9.382	18.777	1.00	96.64	C
ATOM	473	CB	GLN	A	76	10.616	10.469	18.973	1.00	95.93	C
ATOM	474	CG	GLN	A	76	10.033	11.789	19.412	1.00	97.11	C
ATOM	475	CD	GLN	A	76	10.505	12.938	18.547	1.00	99.16	C
ATOM	476	OE1	GLN	A	76	10.410	12.882	17.323	1.00	100.59	O
ATOM	477	NE2	GLN	A	76	11.013	13.990	19.179	1.00	99.62	N
ATOM	478	C	GLN	A	76	10.016	8.426	17.688	1.00	97.19	C
ATOM	479	O	GLN	A	76	10.241	8.837	16.554	1.00	95.99	O
ATOM	480	N	SER	A	77	10.157	7.151	18.025	1.00	99.15	N
ATOM	481	CA	SER	A	77	10.571	6.183	17.024	1.00	102.31	C
ATOM	482	CB	SER	A	77	11.126	4.917	17.677	1.00	102.38	C
ATOM	483	OG	SER	A	77	11.600	4.012	16.694	1.00	100.96	O
ATOM	484	C	SER	A	77	9.351	5.837	16.190	1.00	104.47	C
ATOM	485	O	SER	A	77	9.429	5.773	14.966	1.00	106.20	O
ATOM	486	N	THR	A	78	8.221	5.624	16.857	1.00	105.74	N
ATOM	487	CA	THR	A	78	6.983	5.290	16.166	1.00	107.05	C
ATOM	488	CB	THR	A	78	5.905	4.793	17.143	1.00	108.28	C
ATOM	489	OG1	THR	A	78	5.462	5.883	17.962	1.00	109.87	O
ATOM	490	CG2	THR	A	78	6.464	3.687	18.029	1.00	108.72	C
ATOM	491	C	THR	A	78	6.449	6.519	15.449	1.00	107.78	C
ATOM	492	O	THR	A	78	6.047	6.444	14.293	1.00	108.28	O
ATOM	493	N	LEU	A	79	6.453	7.653	16.143	1.00	109.46	N
ATOM	494	CA	LEU	A	79	5.973	8.912	15.579	1.00	111.76	C
ATOM	495	CB	LEU	A	79	5.859	9.956	16.699	1.00	109.71	C
ATOM	496	CG	LEU	A	79	5.257	11.342	16.435	1.00	108.76	C
ATOM	497	CD1	LEU	A	79	4.667	11.875	17.734	1.00	109.11	C
ATOM	498	CD2	LEU	A	79	6.302	12.299	15.890	1.00	106.36	C
ATOM	499	C	LEU	A	79	6.917	9.401	14.478	1.00	114.37	C
ATOM	500	O	LEU	A	79	6.776	10.509	13.962	1.00	114.05	O
ATOM	501	N	ALA	A	80	7.872	8.550	14.115	1.00	118.14	N
ATOM	502	CA	ALA	A	80	8.862	8.872	13.093	1.00	121.02	C

299/396

Figure 3B-10

ATOM	503	CB	ALA	A	80	10.266	8.720	13.669	1.00	121.24	C
ATOM	504	C	ALA	A	80	8.716	7.981	11.873	1.00	122.67	C
ATOM	505	O	ALA	A	80	8.761	8.452	10.740	1.00	123.48	O
ATOM	506	N	GLN	A	81	8.566	6.685	12.128	1.00	124.92	N
ATOM	507	CA	GLN	A	81	8.416	5.680	11.087	1.00	127.58	C
ATOM	508	CB	GLN	A	81	8.493	4.285	11.718	1.00	126.56	C
ATOM	509	CG	GLN	A	81	7.662	4.173	12.977	1.00	127.61	C
ATOM	510	CD	GLN	A	81	8.245	3.220	14.004	1.00	128.34	C
ATOM	511	OE1	GLN	A	81	9.423	3.306	14.358	1.00	128.95	O
ATOM	512	NE2	GLN	A	81	7.414	2.311	14.498	1.00	128.90	N
ATOM	513	C	GLN	A	81	7.100	5.878	10.334	1.00	129.89	C
ATOM	514	O	GLN	A	81	6.815	5.169	9.364	1.00	130.19	O
ATOM	515	N	MET	A	82	6.302	6.849	10.784	1.00	132.22	N
ATOM	516	CA	MET	A	82	5.033	7.163	10.131	1.00	133.96	C
ATOM	517	CB	MET	A	82	4.299	8.278	10.899	1.00	134.14	C
ATOM	518	CG	MET	A	82	2.957	8.736	10.296	1.00	135.69	C
ATOM	519	SD	MET	A	82	3.059	10.055	9.028	1.00	138.11	S
ATOM	520	CE	MET	A	82	2.510	11.507	9.954	1.00	136.52	C
ATOM	521	C	MET	A	82	5.368	7.616	8.709	1.00	134.87	C
ATOM	522	O	MET	A	82	4.519	7.603	7.816	1.00	136.01	O
ATOM	523	N	TYR	A	83	6.626	8.004	8.512	1.00	134.76	N
ATOM	524	CA	TYR	A	83	7.113	8.460	7.216	1.00	134.68	C
ATOM	525	CB	TYR	A	83	8.179	9.544	7.400	1.00	131.89	C
ATOM	526	CG	TYR	A	83	7.722	10.773	8.159	1.00	128.61	C
ATOM	527	CD1	TYR	A	83	7.276	10.681	9.472	1.00	127.56	C
ATOM	528	CE1	TYR	A	83	6.898	11.803	10.179	1.00	125.49	C
ATOM	529	CD2	TYR	A	83	7.771	12.031	7.575	1.00	126.30	C
ATOM	530	CE2	TYR	A	83	7.395	13.156	8.277	1.00	124.47	C
ATOM	531	CZ	TYR	A	83	6.959	13.037	9.578	1.00	124.34	C
ATOM	532	OH	TYR	A	83	6.582	14.151	10.286	1.00	122.35	O
ATOM	533	C	TYR	A	83	7.724	7.284	6.459	1.00	136.51	C
ATOM	534	O	TYR	A	83	8.636	6.624	6.955	1.00	136.39	O
ATOM	535	N	PRO	A	84	7.236	7.020	5.236	1.00	138.66	N
ATOM	536	CD	PRO	A	84	6.288	7.858	4.482	1.00	139.33	C
ATOM	537	CA	PRO	A	84	7.730	5.919	4.403	1.00	140.01	C
ATOM	538	CB	PRO	A	84	6.886	6.045	3.135	1.00	140.23	C
ATOM	539	CG	PRO	A	84	6.631	7.518	3.052	1.00	139.91	C
ATOM	540	C	PRO	A	84	9.230	5.989	4.120	1.00	141.09	C
ATOM	541	O	PRO	A	84	9.844	7.053	4.214	1.00	140.75	O
ATOM	542	N	LEU	A	85	9.808	4.843	3.774	1.00	142.57	N
ATOM	543	CA	LEU	A	85	11.233	4.745	3.477	1.00	144.59	C
ATOM	544	CB	LEU	A	85	11.548	3.387	2.833	1.00	144.64	C
ATOM	545	CG	LEU	A	85	10.754	2.932	1.602	1.00	144.06	C
ATOM	546	CD1	LEU	A	85	11.511	1.822	0.896	1.00	143.46	C
ATOM	547	CD2	LEU	A	85	9.361	2.472	2.009	1.00	143.96	C
ATOM	548	C	LEU	A	85	11.704	5.869	2.561	1.00	145.91	C
ATOM	549	O	LEU	A	85	12.138	6.923	3.025	1.00	145.67	O
ATOM	550	N	GLN	A	86	11.626	5.628	1.257	1.00	147.90	N
ATOM	551	CA	GLN	A	86	12.026	6.612	0.263	1.00	149.74	C
ATOM	552	CB	GLN	A	86	11.961	5.997	-1.139	1.00	151.05	C
ATOM	553	CG	GLN	A	86	11.211	4.666	-1.215	1.00	153.12	C
ATOM	554	CD	GLN	A	86	9.722	4.786	-0.914	1.00	154.61	C
ATOM	555	OE1	GLN	A	86	9.012	3.781	-0.828	1.00	155.07	O
ATOM	556	NE2	GLN	A	86	9.242	6.015	-0.760	1.00	155.13	N
ATOM	557	C	GLN	A	86	11.111	7.828	0.336	1.00	149.82	C
ATOM	558	O	GLN	A	86	10.924	8.414	1.405	1.00	150.27	O

300/396

Figure 3B-11

ATOM	559	N	GLU	A	87	10.541	8.200	-0.806	1.00	149.19	N
ATOM	560	CA	GLU	A	87	9.639	9.342	-0.878	1.00	148.50	C
ATOM	561	CB	GLU	A	87	8.354	9.053	-0.102	1.00	148.38	C
ATOM	562	CG	GLU	A	87	7.150	9.832	-0.591	1.00	146.65	C
ATOM	563	CD	GLU	A	87	6.542	9.225	-1.839	1.00	145.39	C
ATOM	564	OE1	GLU	A	87	7.240	9.140	-2.872	1.00	144.93	O
ATOM	565	OE2	GLU	A	87	5.361	8.827	-1.782	1.00	144.71	O
ATOM	566	C	GLU	A	87	10.335	10.548	-0.265	1.00	147.88	C
ATOM	567	O	GLU	A	87	9.688	11.506	0.157	1.00	147.95	O
ATOM	568	N	ILE	A	88	11.660	10.481	-0.214	1.00	146.68	N
ATOM	569	CA	ILE	A	88	12.466	11.549	0.351	1.00	145.51	C
ATOM	570	CB	ILE	A	88	12.848	11.241	1.811	1.00	145.57	C
ATOM	571	CG2	ILE	A	88	11.625	11.335	2.704	1.00	145.09	C
ATOM	572	CG1	ILE	A	88	13.484	9.852	1.890	1.00	145.55	C
ATOM	573	CD1	ILE	A	88	13.769	9.396	3.295	1.00	145.21	C
ATOM	574	C	ILE	A	88	13.745	11.748	-0.447	1.00	144.65	C
ATOM	575	O	ILE	A	88	14.548	10.822	-0.592	1.00	144.75	O
ATOM	576	N	GLN	A	89	13.932	12.959	-0.965	1.00	143.53	N
ATOM	577	CA	GLN	A	89	15.129	13.301	-1.739	1.00	142.38	C
ATOM	578	CB	GLN	A	89	14.764	14.308	-2.839	1.00	143.85	C
ATOM	579	CG	GLN	A	89	13.678	13.836	-3.818	1.00	145.20	C
ATOM	580	CD	GLN	A	89	13.359	14.866	-4.891	1.00	146.05	C
ATOM	581	OE1	GLN	A	89	14.202	15.184	-5.731	1.00	145.75	O
ATOM	582	NE2	GLN	A	89	12.139	15.397	-4.863	1.00	146.04	N
ATOM	583	C	GLN	A	89	16.205	13.880	-0.790	1.00	141.08	C
ATOM	584	O	GLN	A	89	16.308	13.430	0.354	1.00	141.08	O
ATOM	585	N	ASN	A	90	16.980	14.868	-1.262	1.00	139.32	N
ATOM	586	CA	ASN	A	90	18.077	15.521	-0.501	1.00	136.74	C
ATOM	587	CB	ASN	A	90	17.576	16.810	0.211	1.00	133.09	C
ATOM	588	CG	ASN	A	90	18.705	17.625	0.892	1.00	129.30	C
ATOM	589	OD1	ASN	A	90	19.847	17.627	0.443	1.00	128.19	O
ATOM	590	ND2	ASN	A	90	18.359	18.337	1.968	1.00	126.50	N
ATOM	591	C	ASN	A	90	18.740	14.576	0.496	1.00	136.95	C
ATOM	592	O	ASN	A	90	18.700	14.796	1.707	1.00	136.63	O
ATOM	593	N	LEU	A	91	19.333	13.517	-0.054	1.00	136.65	N
ATOM	594	CA	LEU	A	91	20.050	12.464	0.675	1.00	135.31	C
ATOM	595	CB	LEU	A	91	21.482	12.369	0.136	1.00	135.84	C
ATOM	596	CG	LEU	A	91	22.017	13.596	-0.611	1.00	135.85	C
ATOM	597	CD1	LEU	A	91	21.222	13.831	-1.898	1.00	134.71	C
ATOM	598	CD2	LEU	A	91	21.954	14.812	0.296	1.00	136.28	C
ATOM	599	C	LEU	A	91	20.082	12.537	2.200	1.00	133.91	C
ATOM	600	O	LEU	A	91	19.624	11.620	2.879	1.00	133.95	O
ATOM	601	N	THR	A	92	20.649	13.616	2.727	1.00	132.22	N
ATOM	602	CA	THR	A	92	20.749	13.826	4.166	1.00	130.22	C
ATOM	603	CB	THR	A	92	21.164	15.276	4.471	1.00	130.60	C
ATOM	604	OG1	THR	A	92	22.539	15.465	4.114	1.00	131.53	O
ATOM	605	CG2	THR	A	92	20.958	15.600	5.945	1.00	128.43	C
ATOM	606	C	THR	A	92	19.438	13.535	4.893	1.00	128.61	C
ATOM	607	O	THR	A	92	19.322	12.534	5.601	1.00	129.42	O
ATOM	608	N	VAL	A	93	18.458	14.417	4.717	1.00	125.69	N
ATOM	609	CA	VAL	A	93	17.159	14.265	5.366	1.00	122.13	C
ATOM	610	CB	VAL	A	93	16.063	15.057	4.609	1.00	122.10	C
ATOM	611	CG1	VAL	A	93	16.260	16.549	4.816	1.00	120.24	C
ATOM	612	CG2	VAL	A	93	16.116	14.732	3.127	1.00	122.17	C
ATOM	613	C	VAL	A	93	16.732	12.802	5.491	1.00	119.67	C
ATOM	614	O	VAL	A	93	16.085	12.417	6.463	1.00	118.26	O

301/396

Figure 3B-12

ATOM	615	N	LYS	A	94	17.115	11.998	4.503	1.00	118.45	N
ATOM	616	CA	LYS	A	94	16.795	10.569	4.453	1.00	117.13	C
ATOM	617	CB	LYS	A	94	17.025	10.053	3.024	1.00	119.35	C
ATOM	618	CG	LYS	A	94	17.069	8.538	2.860	1.00	118.58	C
ATOM	619	CD	LYS	A	94	17.479	8.179	1.438	1.00	118.34	C
ATOM	620	CE	LYS	A	94	17.877	6.721	1.326	1.00	119.67	C
ATOM	621	NZ	LYS	A	94	18.534	6.411	0.023	1.00	120.50	N
ATOM	622	C	LYS	A	94	17.606	9.733	5.446	1.00	114.05	C
ATOM	623	O	LYS	A	94	17.047	8.979	6.243	1.00	112.57	O
ATOM	624	N	LEU	A	95	18.925	9.859	5.394	1.00	111.26	N
ATOM	625	CA	LEU	A	95	19.772	9.100	6.300	1.00	109.24	C
ATOM	626	CB	LEU	A	95	21.253	9.255	5.913	1.00	110.44	C
ATOM	627	CG	LEU	A	95	21.897	10.636	5.753	1.00	109.65	C
ATOM	628	CD1	LEU	A	95	22.114	11.286	7.106	1.00	108.86	C
ATOM	629	CD2	LEU	A	95	23.228	10.471	5.044	1.00	109.83	C
ATOM	630	C	LEU	A	95	19.545	9.530	7.741	1.00	106.39	C
ATOM	631	O	LEU	A	95	19.661	8.724	8.666	1.00	106.77	O
ATOM	632	N	GLN	A	96	19.215	10.803	7.929	1.00	102.90	N
ATOM	633	CA	GLN	A	96	18.966	11.316	9.266	1.00	99.74	C
ATOM	634	CB	GLN	A	96	18.717	12.825	9.218	1.00	95.70	C
ATOM	635	CG	GLN	A	96	19.223	13.557	10.448	1.00	92.95	C
ATOM	636	CD	GLN	A	96	19.175	15.066	10.302	1.00	92.07	C
ATOM	637	OE1	GLN	A	96	19.599	15.622	9.287	1.00	89.38	O
ATOM	638	NE2	GLN	A	96	18.670	15.739	11.327	1.00	92.38	N
ATOM	639	C	GLN	A	96	17.730	10.583	9.761	1.00	99.24	C
ATOM	640	O	GLN	A	96	17.641	10.181	10.922	1.00	99.69	O
ATOM	641	N	LEU	A	97	16.789	10.393	8.845	1.00	97.53	N
ATOM	642	CA	LEU	A	97	15.547	9.702	9.139	1.00	96.44	C
ATOM	643	CB	LEU	A	97	14.660	9.706	7.890	1.00	98.37	C
ATOM	644	CG	LEU	A	97	13.133	9.675	8.012	1.00	98.85	C
ATOM	645	CD1	LEU	A	97	12.683	8.373	8.633	1.00	98.82	C
ATOM	646	CD2	LEU	A	97	12.664	10.864	8.838	1.00	98.00	C
ATOM	647	C	LEU	A	97	15.881	8.272	9.547	1.00	95.12	C
ATOM	648	O	LEU	A	97	15.338	7.755	10.520	1.00	93.42	O
ATOM	649	N	GLN	A	98	16.792	7.652	8.795	1.00	95.87	N
ATOM	650	CA	GLN	A	98	17.232	6.272	9.034	1.00	95.59	C
ATOM	651	CB	GLN	A	98	18.577	6.008	8.350	1.00	95.34	C
ATOM	652	CG	GLN	A	98	18.511	5.898	6.838	1.00	96.62	C
ATOM	653	CD	GLN	A	98	19.868	5.618	6.214	1.00	96.02	C
ATOM	654	OE1	GLN	A	98	20.583	4.717	6.647	1.00	97.86	O
ATOM	655	NE2	GLN	A	98	20.223	6.383	5.188	1.00	94.03	N
ATOM	656	C	GLN	A	98	17.372	5.933	10.504	1.00	95.20	C
ATOM	657	O	GLN	A	98	16.716	5.020	11.008	1.00	93.99	O
ATOM	658	N	ALA	A	99	18.248	6.667	11.179	1.00	95.62	N
ATOM	659	CA	ALA	A	99	18.499	6.456	12.594	1.00	97.06	C
ATOM	660	CB	ALA	A	99	19.286	7.625	13.156	1.00	94.39	C
ATOM	661	C	ALA	A	99	17.190	6.295	13.353	1.00	99.57	C
ATOM	662	O	ALA	A	99	16.864	5.200	13.820	1.00	101.24	O
ATOM	663	N	LEU	A	100	16.440	7.391	13.451	1.00	100.70	N
ATOM	664	CA	LEU	A	100	15.165	7.432	14.166	1.00	100.36	C
ATOM	665	CB	LEU	A	100	14.449	8.746	13.863	1.00	98.93	C
ATOM	666	CG	LEU	A	100	15.008	9.968	14.591	1.00	98.35	C
ATOM	667	CD1	LEU	A	100	14.163	11.192	14.285	1.00	97.26	C
ATOM	668	CD2	LEU	A	100	15.012	9.697	16.085	1.00	98.34	C
ATOM	669	C	LEU	A	100	14.191	6.275	13.960	1.00	102.04	C
ATOM	670	O	LEU	A	100	13.657	5.738	14.935	1.00	101.97	O

302/396

Figure 3B-13

ATOM	671	N	GLN	A	101	13.943	5.897	12.707	1.00	103.55	N
ATOM	672	CA	GLN	A	101	13.014	4.804	12.430	1.00	105.03	C
ATOM	673	CB	GLN	A	101	12.994	4.469	10.937	1.00	103.53	C
ATOM	674	CG	GLN	A	101	12.333	5.536	10.080	1.00	104.26	C
ATOM	675	CD	GLN	A	101	12.094	5.089	8.645	1.00	105.26	C
ATOM	676	OE1	GLN	A	101	11.320	4.165	8.393	1.00	106.32	O
ATOM	677	NE2	GLN	A	101	12.759	5.743	7.698	1.00	103.42	N
ATOM	678	C	GLN	A	101	13.360	3.556	13.236	1.00	106.56	C
ATOM	679	O	GLN	A	101	12.473	2.897	13.786	1.00	106.98	O
ATOM	680	N	GLN	A	102	14.648	3.240	13.318	1.00	106.87	N
ATOM	681	CA	GLN	A	102	15.084	2.068	14.059	1.00	107.55	C
ATOM	682	CB	GLN	A	102	16.595	1.877	13.890	1.00	108.30	C
ATOM	683	CG	GLN	A	102	17.011	1.600	12.451	1.00	110.64	C
ATOM	684	CD	GLN	A	102	18.444	1.118	12.334	1.00	112.77	C
ATOM	685	OE1	GLN	A	102	19.372	1.767	12.818	1.00	114.30	O
ATOM	686	NE2	GLN	A	102	18.633	-0.025	11.685	1.00	112.84	N
ATOM	687	C	GLN	A	102	14.727	2.180	15.537	1.00	107.13	C
ATOM	688	O	GLN	A	102	15.192	3.091	16.214	1.00	106.58	O
ATOM	689	N	ASN	A	103	13.890	1.268	16.030	1.00	108.58	N
ATOM	690	CA	ASN	A	103	13.501	1.279	17.440	1.00	110.82	C
ATOM	691	CB	ASN	A	103	12.478	0.175	17.772	1.00	113.14	C
ATOM	692	CG	ASN	A	103	11.662	-0.294	16.563	1.00	115.36	C
ATOM	693	OD1	ASN	A	103	12.004	-1.281	15.942	1.00	115.79	O
ATOM	694	ND2	ASN	A	103	10.586	0.418	16.235	1.00	116.29	N
ATOM	695	C	ASN	A	103	14.764	0.989	18.234	1.00	110.71	C
ATOM	696	O	ASN	A	103	15.466	0.026	17.933	1.00	111.72	O
ATOM	697	N	GLY	A	104	15.056	1.806	19.240	1.00	110.59	N
ATOM	698	CA	GLY	A	104	16.255	1.583	20.033	1.00	109.63	C
ATOM	699	C	GLY	A	104	16.208	0.256	20.772	1.00	107.96	C
ATOM	700	O	GLY	A	104	15.604	-0.708	20.305	1.00	106.15	O
ATOM	701	N	SER	A	105	16.847	0.197	21.933	1.00	107.18	N
ATOM	702	CA	SER	A	105	16.837	-1.026	22.720	1.00	105.46	C
ATOM	703	CB	SER	A	105	17.910	-0.958	23.823	1.00	107.26	C
ATOM	704	OG	SER	A	105	18.333	-2.250	24.243	1.00	105.92	O
ATOM	705	C	SER	A	105	15.436	-1.140	23.327	1.00	102.66	C
ATOM	706	O	SER	A	105	15.228	-1.836	24.321	1.00	102.22	O
ATOM	707	N	SER	A	106	14.483	-0.432	22.724	1.00	100.13	N
ATOM	708	CA	SER	A	106	13.091	-0.446	23.179	1.00	98.23	C
ATOM	709	CB	SER	A	106	12.314	0.743	22.592	1.00	98.64	C
ATOM	710	OG	SER	A	106	12.239	0.675	21.176	1.00	98.31	O
ATOM	711	C	SER	A	106	12.482	-1.753	22.696	1.00	95.43	C
ATOM	712	O	SER	A	106	11.476	-2.235	23.227	1.00	92.99	O
ATOM	713	N	VAL	A	107	13.129	-2.312	21.679	1.00	92.74	N
ATOM	714	CA	VAL	A	107	12.736	-3.572	21.070	1.00	89.96	C
ATOM	715	CB	VAL	A	107	13.774	-3.996	20.008	1.00	90.37	C
ATOM	716	CG1	VAL	A	107	13.397	-5.320	19.405	1.00	91.02	C
ATOM	717	CG2	VAL	A	107	13.864	-2.938	18.922	1.00	91.17	C
ATOM	718	C	VAL	A	107	12.657	-4.635	22.159	1.00	87.76	C
ATOM	719	O	VAL	A	107	12.187	-5.751	21.930	1.00	87.16	O
ATOM	720	N	LEU	A	108	13.120	-4.270	23.349	1.00	85.74	N
ATOM	721	CA	LEU	A	108	13.112	-5.170	24.489	1.00	84.41	C
ATOM	722	CB	LEU	A	108	14.329	-4.924	25.382	1.00	81.70	C
ATOM	723	CG	LEU	A	108	15.677	-5.429	24.880	1.00	79.34	C
ATOM	724	CD1	LEU	A	108	16.792	-4.679	25.565	1.00	81.61	C
ATOM	725	CD2	LEU	A	108	15.788	-6.908	25.136	1.00	78.73	C
ATOM	726	C	LEU	A	108	11.853	-4.999	25.310	1.00	85.92	C

303/396

Figure 3B-14

ATOM	727	O	LEU	A	108	11.163	-3.974	25.233	1.00	83.94	O
ATOM	728	N	SER	A	109	11.578	-6.027	26.104	1.00	88.09	N
ATOM	729	CA	SER	A	109	10.418	-6.076	26.972	1.00	89.75	C
ATOM	730	CB	SER	A	109	10.346	-7.444	27.644	1.00	88.51	C
ATOM	731	OG	SER	A	109	9.570	-7.393	28.823	1.00	86.99	O
ATOM	732	C	SER	A	109	10.439	-4.998	28.036	1.00	92.92	C
ATOM	733	O	SER	A	109	10.650	-5.302	29.205	1.00	94.26	O
ATOM	734	N	GLU	A	110	10.221	-3.747	27.630	1.00	96.07	N
ATOM	735	CA	GLU	A	110	10.190	-2.617	28.559	1.00	98.50	C
ATOM	736	CB	GLU	A	110	8.736	-2.136	28.723	1.00	101.51	C
ATOM	737	CG	GLU	A	110	8.424	-1.324	29.981	1.00	105.62	C
ATOM	738	CD	GLU	A	110	9.382	-0.172	30.199	1.00	109.27	C
ATOM	739	OE1	GLU	A	110	9.750	0.490	29.205	1.00	111.14	O
ATOM	740	OE2	GLU	A	110	9.759	0.076	31.367	1.00	110.68	O
ATOM	741	C	GLU	A	110	10.802	-2.973	29.916	1.00	97.95	C
ATOM	742	O	GLU	A	110	11.979	-2.711	30.163	1.00	98.23	O
ATOM	743	N	ASP	A	111	10.007	-3.589	30.783	1.00	96.66	N
ATOM	744	CA	ASP	A	111	10.477	-3.974	32.102	1.00	96.88	C
ATOM	745	CB	ASP	A	111	9.283	-4.272	33.006	1.00	99.52	C
ATOM	746	CG	ASP	A	111	8.502	-3.018	33.354	1.00	100.93	C
ATOM	747	OD1	ASP	A	111	9.099	-2.098	33.962	1.00	101.23	O
ATOM	748	OD2	ASP	A	111	7.300	-2.950	33.017	1.00	100.98	O
ATOM	749	C	ASP	A	111	11.441	-5.153	32.075	1.00	95.78	C
ATOM	750	O	ASP	A	111	11.436	-6.006	32.963	1.00	95.74	O
ATOM	751	N	LYS	A	112	12.264	-5.186	31.035	1.00	95.27	N
ATOM	752	CA	LYS	A	112	13.281	-6.212	30.849	1.00	94.83	C
ATOM	753	CB	LYS	A	112	12.972	-7.087	29.633	1.00	94.32	C
ATOM	754	CG	LYS	A	112	14.208	-7.724	29.035	1.00	93.77	C
ATOM	755	CD	LYS	A	112	13.866	-8.901	28.155	1.00	96.30	C
ATOM	756	CE	LYS	A	112	13.382	-10.094	28.972	1.00	96.04	C
ATOM	757	NZ	LYS	A	112	13.177	-11.305	28.111	1.00	95.98	N
ATOM	758	C	LYS	A	112	14.577	-5.451	30.620	1.00	94.28	C
ATOM	759	O	LYS	A	112	15.591	-5.710	31.267	1.00	95.90	O
ATOM	760	N	SER	A	113	14.529	-4.499	29.695	1.00	91.28	N
ATOM	761	CA	SER	A	113	15.682	-3.669	29.403	1.00	88.13	C
ATOM	762	CB	SER	A	113	15.280	-2.551	28.441	1.00	88.71	C
ATOM	763	OG	SER	A	113	14.086	-1.919	28.866	1.00	86.37	O
ATOM	764	C	SER	A	113	16.183	-3.084	30.724	1.00	86.89	C
ATOM	765	O	SER	A	113	17.334	-2.661	30.836	1.00	85.90	O
ATOM	766	N	LYS	A	114	15.305	-3.066	31.725	1.00	85.25	N
ATOM	767	CA	LYS	A	114	15.667	-2.557	33.037	1.00	83.05	C
ATOM	768	CB	LYS	A	114	14.484	-2.622	34.013	1.00	82.60	C
ATOM	769	CG	LYS	A	114	13.299	-1.726	33.642	1.00	84.03	C
ATOM	770	CD	LYS	A	114	12.430	-1.350	34.854	1.00	82.59	C
ATOM	771	CE	LYS	A	114	11.895	-2.563	35.601	1.00	80.40	C
ATOM	772	NZ	LYS	A	114	12.981	-3.394	36.192	1.00	77.02	N
ATOM	773	C	LYS	A	114	16.807	-3.404	33.565	1.00	81.53	C
ATOM	774	O	LYS	A	114	17.816	-2.873	34.018	1.00	84.47	O
ATOM	775	N	ARG	A	115	16.659	-4.722	33.500	1.00	79.26	N
ATOM	776	CA	ARG	A	115	17.715	-5.599	33.981	1.00	77.74	C
ATOM	777	CB	ARG	A	115	17.344	-7.062	33.791	1.00	78.71	C
ATOM	778	CG	ARG	A	115	18.410	-8.021	34.303	1.00	81.41	C
ATOM	779	CD	ARG	A	115	18.402	-8.106	35.824	1.00	84.06	C
ATOM	780	NE	ARG	A	115	19.424	-9.018	36.333	1.00	84.92	N
ATOM	781	CZ	ARG	A	115	20.633	-8.638	36.737	1.00	84.83	C
ATOM	782	NH1	ARG	A	115	21.504	-9.535	37.182	1.00	84.33	N

304/396

Figure 3B-15

ATOM	783	NH2	ARG	A	115	20.967	-7.357	36.712	1.00	84.75	N
ATOM	784	C	ARG	A	115	19.017	-5.312	33.241	1.00	77.02	C
ATOM	785	O	ARG	A	115	20.095	-5.447	33.811	1.00	78.10	O
ATOM	786	N	LEU	A	116	18.923	-4.924	31.972	1.00	75.34	N
ATOM	787	CA	LEU	A	116	20.124	-4.608	31.205	1.00	72.54	C
ATOM	788	CB	LEU	A	116	19.783	-4.199	29.772	1.00	69.50	C
ATOM	789	CG	LEU	A	116	20.978	-3.902	28.857	1.00	64.93	C
ATOM	790	CD1	LEU	A	116	21.877	-5.132	28.753	1.00	61.28	C
ATOM	791	CD2	LEU	A	116	20.475	-3.482	27.483	1.00	63.23	C
ATOM	792	C	LEU	A	116	20.799	-3.449	31.908	1.00	73.51	C
ATOM	793	O	LEU	A	116	21.978	-3.525	32.243	1.00	76.00	O
ATOM	794	N	ASN	A	117	20.049	-2.375	32.134	1.00	72.20	N
ATOM	795	CA	ASN	A	117	20.597	-1.215	32.821	1.00	72.22	C
ATOM	796	CB	ASN	A	117	19.519	-0.167	33.026	1.00	76.19	C
ATOM	797	CG	ASN	A	117	19.009	0.376	31.720	1.00	83.40	C
ATOM	798	OD1	ASN	A	117	18.211	1.315	31.685	1.00	90.28	O
ATOM	799	ND2	ASN	A	117	19.469	-0.216	30.624	1.00	85.60	N
ATOM	800	C	ASN	A	117	21.169	-1.647	34.156	1.00	70.58	C
ATOM	801	O	ASN	A	117	22.325	-1.365	34.461	1.00	71.02	O
ATOM	802	N	THR	A	118	20.359	-2.334	34.949	1.00	68.45	N
ATOM	803	CA	THR	A	118	20.806	-2.836	36.240	1.00	68.01	C
ATOM	804	CB	THR	A	118	19.830	-3.875	36.782	1.00	67.78	C
ATOM	805	OG1	THR	A	118	18.642	-3.225	37.239	1.00	68.15	O
ATOM	806	CG2	THR	A	118	20.463	-4.652	37.910	1.00	69.19	C
ATOM	807	C	THR	A	118	22.165	-3.509	36.066	1.00	67.43	C
ATOM	808	O	THR	A	118	23.127	-3.213	36.773	1.00	67.31	O
ATOM	809	N	ILE	A	119	22.222	-4.426	35.110	1.00	67.06	N
ATOM	810	CA	ILE	A	119	23.440	-5.154	34.793	1.00	65.95	C
ATOM	811	CB	ILE	A	119	23.160	-6.178	33.676	1.00	65.32	C
ATOM	812	CG2	ILE	A	119	24.447	-6.791	33.163	1.00	64.06	C
ATOM	813	CG1	ILE	A	119	22.233	-7.256	34.226	1.00	66.44	C
ATOM	814	CD1	ILE	A	119	21.827	-8.303	33.217	1.00	74.56	C
ATOM	815	C	ILE	A	119	24.536	-4.184	34.356	1.00	64.49	C
ATOM	816	O	ILE	A	119	25.666	-4.245	34.847	1.00	64.64	O
ATOM	817	N	LEU	A	120	24.187	-3.283	33.444	1.00	61.69	N
ATOM	818	CA	LEU	A	120	25.121	-2.292	32.933	1.00	60.75	C
ATOM	819	CB	LEU	A	120	24.439	-1.411	31.891	1.00	57.65	C
ATOM	820	CG	LEU	A	120	24.436	-2.028	30.503	1.00	56.17	C
ATOM	821	CD1	LEU	A	120	24.228	-0.954	29.467	1.00	56.08	C
ATOM	822	CD2	LEU	A	120	25.777	-2.719	30.276	1.00	57.83	C
ATOM	823	C	LEU	A	120	25.731	-1.404	34.005	1.00	60.97	C
ATOM	824	O	LEU	A	120	26.951	-1.231	34.050	1.00	60.19	O
ATOM	825	N	ASN	A	121	24.881	-0.834	34.854	1.00	60.80	N
ATOM	826	CA	ASN	A	121	25.345	0.042	35.918	1.00	61.65	C
ATOM	827	CB	ASN	A	121	24.175	0.631	36.695	1.00	63.26	C
ATOM	828	CG	ASN	A	121	23.531	1.780	35.970	1.00	65.46	C
ATOM	829	OD1	ASN	A	121	24.201	2.516	35.247	1.00	70.18	O
ATOM	830	ND2	ASN	A	121	22.232	1.959	36.168	1.00	66.22	N
ATOM	831	C	ASN	A	121	26.269	-0.661	36.878	1.00	61.50	C
ATOM	832	O	ASN	A	121	27.300	-0.103	37.268	1.00	64.75	O
ATOM	833	N	THR	A	122	25.901	-1.876	37.270	1.00	57.77	N
ATOM	834	CA	THR	A	122	26.738	-2.641	38.183	1.00	56.08	C
ATOM	835	CB	THR	A	122	26.212	-4.054	38.407	1.00	57.38	C
ATOM	836	OG1	THR	A	122	24.817	-4.001	38.735	1.00	62.24	O
ATOM	837	CG2	THR	A	122	26.991	-4.732	39.538	1.00	51.16	C
ATOM	838	C	THR	A	122	28.101	-2.775	37.549	1.00	55.20	C

305/396

Figure 3B-16

ATOM	839	O	THR	A	122	29.091	-2.219	38.032	1.00	55.28	O
ATOM	840	N	MET	A	123	28.137	-3.519	36.454	1.00	54.05	N
ATOM	841	CA	MET	A	123	29.369	-3.744	35.724	1.00	55.12	C
ATOM	842	CB	MET	A	123	29.046	-4.014	34.272	1.00	54.95	C
ATOM	843	CG	MET	A	123	28.252	-5.268	34.091	1.00	53.90	C
ATOM	844	SD	MET	A	123	28.994	-6.149	32.768	1.00	53.83	S
ATOM	845	CE	MET	A	123	28.315	-5.221	31.360	1.00	54.23	C
ATOM	846	C	MET	A	123	30.307	-2.560	35.836	1.00	55.44	C
ATOM	847	O	MET	A	123	31.482	-2.720	36.141	1.00	53.87	O
ATOM	848	N	SER	A	124	29.774	-1.371	35.589	1.00	56.72	N
ATOM	849	CA	SER	A	124	30.559	-0.153	35.687	1.00	58.93	C
ATOM	850	CB	SER	A	124	29.713	1.059	35.329	1.00	58.44	C
ATOM	851	OG	SER	A	124	30.286	2.225	35.895	1.00	60.10	O
ATOM	852	C	SER	A	124	31.094	0.044	37.100	1.00	59.58	C
ATOM	853	O	SER	A	124	32.312	0.134	37.316	1.00	58.32	O
ATOM	854	N	THR	A	125	30.178	0.131	38.062	1.00	57.30	N
ATOM	855	CA	THR	A	125	30.595	0.339	39.436	1.00	57.24	C
ATOM	856	CB	THR	A	125	29.413	0.261	40.428	1.00	57.24	C
ATOM	857	OG1	THR	A	125	29.155	-1.104	40.769	1.00	58.03	O
ATOM	858	CG2	THR	A	125	28.167	0.896	39.814	1.00	53.79	C
ATOM	859	C	THR	A	125	31.649	-0.691	39.800	1.00	55.14	C
ATOM	860	O	THR	A	125	32.749	-0.321	40.193	1.00	55.58	O
ATOM	861	N	ILE	A	126	31.330	-1.975	39.643	1.00	53.09	N
ATOM	862	CA	ILE	A	126	32.294	-3.034	39.961	1.00	51.17	C
ATOM	863	CB	ILE	A	126	31.938	-4.373	39.270	1.00	46.52	C
ATOM	864	CG2	ILE	A	126	33.023	-5.394	39.533	1.00	43.13	C
ATOM	865	CG1	ILE	A	126	30.629	-4.918	39.821	1.00	44.38	C
ATOM	866	CD1	ILE	A	126	30.709	-5.262	41.266	1.00	48.15	C
ATOM	867	C	ILE	A	126	33.696	-2.624	39.509	1.00	50.42	C
ATOM	868	O	ILE	A	126	34.637	-2.610	40.289	1.00	49.71	O
ATOM	869	N	TYR	A	127	33.815	-2.269	38.242	1.00	49.90	N
ATOM	870	CA	TYR	A	127	35.085	-1.858	37.685	1.00	50.22	C
ATOM	871	CB	TYR	A	127	34.903	-1.474	36.214	1.00	50.26	C
ATOM	872	CG	TYR	A	127	36.192	-1.231	35.474	1.00	49.26	C
ATOM	873	CD1	TYR	A	127	36.618	0.053	35.177	1.00	45.53	C
ATOM	874	CE1	TYR	A	127	37.796	0.267	34.500	1.00	45.83	C
ATOM	875	CD2	TYR	A	127	36.988	-2.297	35.072	1.00	52.15	C
ATOM	876	CE2	TYR	A	127	38.173	-2.091	34.394	1.00	51.27	C
ATOM	877	CZ	TYR	A	127	38.569	-0.807	34.112	1.00	48.78	C
ATOM	878	OH	TYR	A	127	39.745	-0.610	33.439	1.00	50.53	O
ATOM	879	C	TYR	A	127	35.659	-0.684	38.456	1.00	52.62	C
ATOM	880	O	TYR	A	127	36.680	-0.815	39.119	1.00	56.25	O
ATOM	881	N	SER	A	128	35.000	0.466	38.375	1.00	53.33	N
ATOM	882	CA	SER	A	128	35.487	1.659	39.053	1.00	51.95	C
ATOM	883	CB	SER	A	128	34.977	2.902	38.342	1.00	50.51	C
ATOM	884	OG	SER	A	128	35.247	2.810	36.960	1.00	53.61	O
ATOM	885	C	SER	A	128	35.026	1.696	40.484	1.00	52.34	C
ATOM	886	O	SER	A	128	34.268	2.584	40.851	1.00	57.36	O
ATOM	887	N	THR	A	129	35.488	0.752	41.297	1.00	50.30	N
ATOM	888	CA	THR	A	129	35.075	0.680	42.698	1.00	47.57	C
ATOM	889	CB	THR	A	129	33.525	0.641	42.823	1.00	47.90	C
ATOM	890	OG1	THR	A	129	33.024	1.940	43.155	1.00	41.89	O
ATOM	891	CG2	THR	A	129	33.098	-0.334	43.863	1.00	46.87	C
ATOM	892	C	THR	A	129	35.641	-0.582	43.306	1.00	47.02	C
ATOM	893	O	THR	A	129	35.923	-0.647	44.492	1.00	47.08	O
ATOM	894	N	GLY	A	130	35.803	-1.594	42.472	1.00	50.74	N

306/396

Figure 3B-17

ATOM	895	CA	GLY	A	130	36.347	-2.858	42.937	1.00	52.50	C
ATOM	896	C	GLY	A	130	37.697	-2.723	43.606	1.00	49.60	C
ATOM	897	O	GLY	A	130	38.520	-1.903	43.219	1.00	46.15	O
ATOM	898	N	LYS	A	131	37.926	-3.543	44.617	1.00	52.43	N
ATOM	899	CA	LYS	A	131	39.188	-3.485	45.324	1.00	59.36	C
ATOM	900	CB	LYS	A	131	39.004	-2.766	46.666	1.00	64.14	C
ATOM	901	CG	LYS	A	131	38.329	-1.413	46.595	1.00	66.21	C
ATOM	902	CD	LYS	A	131	38.763	-0.538	47.763	1.00	68.86	C
ATOM	903	CE	LYS	A	131	38.122	0.850	47.700	1.00	71.97	C
ATOM	904	NZ	LYS	A	131	38.675	1.826	48.700	1.00	73.53	N
ATOM	905	C	LYS	A	131	39.790	-4.857	45.601	1.00	60.94	C
ATOM	906	O	LYS	A	131	39.071	-5.841	45.789	1.00	61.29	O
ATOM	907	N	VAL	A	132	41.115	-4.922	45.599	1.00	61.44	N
ATOM	908	CA	VAL	A	132	41.802	-6.156	45.947	1.00	67.06	C
ATOM	909	CB	VAL	A	132	42.798	-6.647	44.865	1.00	65.74	C
ATOM	910	CG1	VAL	A	132	42.046	-7.124	43.639	1.00	66.12	C
ATOM	911	CG2	VAL	A	132	43.767	-5.551	44.510	1.00	67.11	C
ATOM	912	C	VAL	A	132	42.568	-5.722	47.183	1.00	70.34	C
ATOM	913	O	VAL	A	132	43.194	-4.663	47.183	1.00	71.68	O
ATOM	914	N	CYS	A	133	42.501	-6.509	48.250	1.00	73.75	N
ATOM	915	CA	CYS	A	133	43.194	-6.125	49.465	1.00	74.08	C
ATOM	916	C	CYS	A	133	44.434	-6.965	49.752	1.00	71.60	C
ATOM	917	O	CYS	A	133	44.433	-8.180	49.588	1.00	69.02	O
ATOM	918	CB	CYS	A	133	42.224	-6.152	50.645	1.00	76.88	C
ATOM	919	SG	CYS	A	133	42.460	-4.710	51.740	1.00	88.22	S
ATOM	920	N	ASN	A	134	45.499	-6.283	50.161	1.00	69.69	N
ATOM	921	CA	ASN	A	134	46.767	-6.915	50.469	1.00	70.26	C
ATOM	922	CB	ASN	A	134	47.647	-5.945	51.239	1.00	66.20	C
ATOM	923	CG	ASN	A	134	49.031	-6.485	51.469	1.00	65.47	C
ATOM	924	OD1	ASN	A	134	49.203	-7.665	51.759	1.00	61.13	O
ATOM	925	ND2	ASN	A	134	50.031	-5.622	51.354	1.00	63.72	N
ATOM	926	C	ASN	A	134	46.543	-8.163	51.306	1.00	74.15	C
ATOM	927	O	ASN	A	134	45.806	-8.127	52.287	1.00	77.43	O
ATOM	928	N	PRO	A	135	47.189	-9.284	50.938	1.00	76.66	N
ATOM	929	CD	PRO	A	135	48.106	-9.436	49.797	1.00	78.31	C
ATOM	930	CA	PRO	A	135	47.058	-10.558	51.656	1.00	76.76	C
ATOM	931	CB	PRO	A	135	47.933	-11.512	50.841	1.00	77.98	C
ATOM	932	CG	PRO	A	135	47.954	-10.901	49.481	1.00	78.11	C
ATOM	933	C	PRO	A	135	47.563	-10.436	53.080	1.00	76.12	C
ATOM	934	O	PRO	A	135	46.864	-10.752	54.039	1.00	74.05	O
ATOM	935	N	ASP	A	136	48.797	-9.964	53.187	1.00	76.51	N
ATOM	936	CA	ASP	A	136	49.466	-9.787	54.458	1.00	76.57	C
ATOM	937	CB	ASP	A	136	50.969	-9.712	54.228	1.00	80.28	C
ATOM	938	CG	ASP	A	136	51.342	-8.643	53.223	1.00	85.63	C
ATOM	939	OD1	ASP	A	136	51.152	-8.870	52.008	1.00	87.80	O
ATOM	940	OD2	ASP	A	136	51.810	-7.565	53.649	1.00	89.73	O
ATOM	941	C	ASP	A	136	49.016	-8.544	55.217	1.00	74.95	C
ATOM	942	O	ASP	A	136	49.766	-8.040	56.051	1.00	76.88	O
ATOM	943	N	ASN	A	137	47.813	-8.047	54.925	1.00	70.95	N
ATOM	944	CA	ASN	A	137	47.260	-6.868	55.610	1.00	66.76	C
ATOM	945	CB	ASN	A	137	48.189	-5.654	55.482	1.00	65.58	C
ATOM	946	CG	ASN	A	137	47.659	-4.429	56.223	1.00	64.40	C
ATOM	947	OD1	ASN	A	137	48.286	-3.377	56.211	1.00	65.33	O
ATOM	948	ND2	ASN	A	137	46.504	-4.565	56.869	1.00	62.91	N
ATOM	949	C	ASN	A	137	45.885	-6.500	55.072	1.00	64.04	C
ATOM	950	O	ASN	A	137	45.728	-5.556	54.300	1.00	65.09	O

307/396

Figure 3B-18

ATOM	951	N	PRO	A	138	44.869	-7.238	55.498	1.00	59.94	N
ATOM	952	CD	PRO	A	138	45.021	-8.236	56.563	1.00	59.88	C
ATOM	953	CA	PRO	A	138	43.465	-7.088	55.130	1.00	60.67	C
ATOM	954	CB	PRO	A	138	42.747	-7.837	56.245	1.00	60.54	C
ATOM	955	CG	PRO	A	138	43.687	-8.930	56.544	1.00	62.08	C
ATOM	956	C	PRO	A	138	42.979	-5.648	55.022	1.00	60.22	C
ATOM	957	O	PRO	A	138	41.865	-5.402	54.557	1.00	58.68	O
ATOM	958	N	GLN	A	139	43.797	-4.697	55.459	1.00	59.77	N
ATOM	959	CA	GLN	A	139	43.380	-3.308	55.409	1.00	60.44	C
ATOM	960	CB	GLN	A	139	43.540	-2.678	56.787	1.00	57.97	C
ATOM	961	CG	GLN	A	139	42.489	-3.199	57.772	1.00	56.40	C
ATOM	962	CD	GLN	A	139	42.815	-4.572	58.336	1.00	56.70	C
ATOM	963	OE1	GLN	A	139	41.919	-5.331	58.694	1.00	54.33	O
ATOM	964	NE2	GLN	A	139	44.104	-4.888	58.436	1.00	54.71	N
ATOM	965	C	GLN	A	139	44.045	-2.465	54.326	1.00	62.58	C
ATOM	966	O	GLN	A	139	43.652	-1.323	54.081	1.00	60.83	O
ATOM	967	N	GLU	A	140	45.043	-3.033	53.661	1.00	64.83	N
ATOM	968	CA	GLU	A	140	45.694	-2.318	52.581	1.00	66.06	C
ATOM	969	CB	GLU	A	140	47.181	-2.664	52.511	1.00	66.79	C
ATOM	970	CG	GLU	A	140	47.999	-1.654	51.718	1.00	73.62	C
ATOM	971	CD	GLU	A	140	49.364	-2.187	51.292	1.00	80.22	C
ATOM	972	OE1	GLU	A	140	50.090	-2.756	52.142	1.00	82.21	O
ATOM	973	OE2	GLU	A	140	49.715	-2.027	50.100	1.00	80.79	O
ATOM	974	C	GLU	A	140	44.986	-2.787	51.312	1.00	66.55	C
ATOM	975	O	GLU	A	140	45.367	-3.795	50.720	1.00	65.77	O
ATOM	976	N	CYS	A	141	43.929	-2.076	50.925	1.00	67.06	N
ATOM	977	CA	CYS	A	141	43.176	-2.415	49.719	1.00	68.01	C
ATOM	978	C	CYS	A	141	43.556	-1.459	48.586	1.00	65.20	C
ATOM	979	O	CYS	A	141	43.924	-0.312	48.821	1.00	64.76	O
ATOM	980	CB	CYS	A	141	41.665	-2.319	49.973	1.00	73.23	C
ATOM	981	SG	CYS	A	141	40.976	-3.380	51.292	1.00	81.57	S
ATOM	982	N	LEU	A	142	43.468	-1.928	47.351	1.00	62.89	N
ATOM	983	CA	LEU	A	142	43.807	-1.081	46.220	1.00	58.75	C
ATOM	984	CB	LEU	A	142	45.148	-1.507	45.623	1.00	54.13	C
ATOM	985	CG	LEU	A	142	46.364	-1.192	46.486	1.00	53.49	C
ATOM	986	CD1	LEU	A	142	47.629	-1.301	45.659	1.00	51.53	C
ATOM	987	CD2	LEU	A	142	46.229	0.207	47.035	1.00	52.06	C
ATOM	988	C	LEU	A	142	42.742	-1.045	45.121	1.00	60.03	C
ATOM	989	O	LEU	A	142	42.240	-2.084	44.652	1.00	60.99	O
ATOM	990	N	LEU	A	143	42.395	0.172	44.725	1.00	55.73	N
ATOM	991	CA	LEU	A	143	41.425	0.398	43.675	1.00	53.40	C
ATOM	992	CB	LEU	A	143	40.986	1.857	43.745	1.00	49.31	C
ATOM	993	CG	LEU	A	143	39.510	2.231	43.849	1.00	44.40	C
ATOM	994	CD1	LEU	A	143	38.777	1.219	44.643	1.00	41.10	C
ATOM	995	CD2	LEU	A	143	39.387	3.599	44.476	1.00	45.16	C
ATOM	996	C	LEU	A	143	42.234	0.126	42.406	1.00	56.76	C
ATOM	997	O	LEU	A	143	43.452	-0.012	42.485	1.00	60.15	O
ATOM	998	N	LEU	A	144	41.598	0.032	41.241	1.00	57.71	N
ATOM	999	CA	LEU	A	144	42.379	-0.203	40.029	1.00	56.17	C
ATOM	1000	CB	LEU	A	144	41.488	-0.643	38.863	1.00	58.74	C
ATOM	1001	CG	LEU	A	144	42.203	-0.813	37.510	1.00	58.82	C
ATOM	1002	CD1	LEU	A	144	43.178	-1.973	37.587	1.00	61.78	C
ATOM	1003	CD2	LEU	A	144	41.192	-1.058	36.406	1.00	58.83	C
ATOM	1004	C	LEU	A	144	43.130	1.071	39.646	1.00	54.78	C
ATOM	1005	O	LEU	A	144	44.115	1.018	38.920	1.00	52.19	O
ATOM	1006	N	GLU	A	145	42.664	2.217	40.134	1.00	54.12	N

308/396

Figure 3B-19

ATOM	1007	CA	GLU	A	145	43.325	3.483	39.833	1.00	55.68	C
ATOM	1008	CB	GLU	A	145	42.616	4.178	38.668	1.00	57.25	C
ATOM	1009	CG	GLU	A	145	42.816	5.688	38.561	1.00	60.68	C
ATOM	1010	CD	GLU	A	145	44.230	6.095	38.202	1.00	67.11	C
ATOM	1011	OE1	GLU	A	145	44.975	5.250	37.651	1.00	69.64	O
ATOM	1012	OE2	GLU	A	145	44.588	7.271	38.455	1.00	68.11	O
ATOM	1013	C	GLU	A	145	43.400	4.427	41.031	1.00	57.13	C
ATOM	1014	O	GLU	A	145	42.393	4.964	41.481	1.00	59.66	O
ATOM	1015	N	PRO	A	146	44.601	4.583	41.604	1.00	57.12	N
ATOM	1016	CD	PRO	A	146	44.988	5.798	42.347	1.00	53.01	C
ATOM	1017	CA	PRO	A	146	45.785	3.871	41.106	1.00	55.60	C
ATOM	1018	CB	PRO	A	146	46.837	4.957	41.053	1.00	51.95	C
ATOM	1019	CG	PRO	A	146	46.510	5.771	42.275	1.00	53.62	C
ATOM	1020	C	PRO	A	146	46.136	2.753	42.090	1.00	57.15	C
ATOM	1021	O	PRO	A	146	45.434	2.531	43.079	1.00	55.51	O
ATOM	1022	N	GLY	A	147	47.224	2.053	41.834	1.00	58.95	N
ATOM	1023	CA	GLY	A	147	47.589	0.971	42.726	1.00	62.18	C
ATOM	1024	C	GLY	A	147	47.731	-0.254	41.860	1.00	64.36	C
ATOM	1025	O	GLY	A	147	48.837	-0.547	41.398	1.00	66.14	O
ATOM	1026	N	LEU	A	148	46.632	-0.971	41.629	1.00	62.14	N
ATOM	1027	CA	LEU	A	148	46.707	-2.127	40.758	1.00	60.52	C
ATOM	1028	CB	LEU	A	148	45.317	-2.661	40.417	1.00	59.60	C
ATOM	1029	CG	LEU	A	148	44.722	-3.728	41.333	1.00	57.78	C
ATOM	1030	CD1	LEU	A	148	45.815	-4.276	42.223	1.00	51.12	C
ATOM	1031	CD2	LEU	A	148	43.581	-3.135	42.146	1.00	54.49	C
ATOM	1032	C	LEU	A	148	47.365	-1.586	39.499	1.00	61.16	C
ATOM	1033	O	LEU	A	148	48.154	-2.266	38.856	1.00	63.56	O
ATOM	1034	N	ASN	A	149	47.046	-0.337	39.174	1.00	60.89	N
ATOM	1035	CA	ASN	A	149	47.594	0.327	38.000	1.00	59.57	C
ATOM	1036	CB	ASN	A	149	46.747	1.557	37.621	1.00	64.52	C
ATOM	1037	CG	ASN	A	149	45.637	1.237	36.600	1.00	64.62	C
ATOM	1038	OD1	ASN	A	149	44.824	2.106	36.255	1.00	61.30	O
ATOM	1039	ND2	ASN	A	149	45.613	-0.006	36.110	1.00	61.95	N
ATOM	1040	C	ASN	A	149	49.047	0.740	38.166	1.00	57.51	C
ATOM	1041	O	ASN	A	149	49.886	0.294	37.398	1.00	57.90	O
ATOM	1042	N	ALA	A	150	49.359	1.584	39.150	1.00	57.62	N
ATOM	1043	CA	ALA	A	150	50.754	2.020	39.334	1.00	57.24	C
ATOM	1044	CB	ALA	A	150	50.909	2.820	40.618	1.00	50.54	C
ATOM	1045	C	ALA	A	150	51.703	0.820	39.349	1.00	58.28	C
ATOM	1046	O	ALA	A	150	52.801	0.871	38.793	1.00	56.61	O
ATOM	1047	N	ILE	A	151	51.256	-0.265	39.975	1.00	57.71	N
ATOM	1048	CA	ILE	A	151	52.039	-1.486	40.069	1.00	55.76	C
ATOM	1049	CB	ILE	A	151	51.376	-2.479	41.031	1.00	57.05	C
ATOM	1050	CG2	ILE	A	151	52.013	-3.851	40.872	1.00	60.52	C
ATOM	1051	CG1	ILE	A	151	51.483	-1.959	42.469	1.00	54.58	C
ATOM	1052	CD1	ILE	A	151	50.768	-2.823	43.488	1.00	49.78	C
ATOM	1053	C	ILE	A	151	52.221	-2.160	38.713	1.00	55.18	C
ATOM	1054	O	ILE	A	151	53.346	-2.367	38.275	1.00	56.09	O
ATOM	1055	N	MET	A	152	51.120	-2.503	38.050	1.00	55.12	N
ATOM	1056	CA	MET	A	152	51.174	-3.146	36.734	1.00	54.29	C
ATOM	1057	CB	MET	A	152	49.768	-3.438	36.224	1.00	53.82	C
ATOM	1058	CG	MET	A	152	49.063	-4.520	36.977	1.00	54.77	C
ATOM	1059	SD	MET	A	152	50.136	-5.926	37.040	1.00	58.78	S
ATOM	1060	CE	MET	A	152	49.820	-6.686	35.476	1.00	56.24	C
ATOM	1061	C	MET	A	152	51.897	-2.295	35.697	1.00	54.39	C
ATOM	1062	O	MET	A	152	52.149	-2.743	34.585	1.00	55.13	O

309/396

Figure 3B-20

ATOM	1063	N	ALA	A	153	52.228	-1.066	36.067	1.00	54.18	N
ATOM	1064	CA	ALA	A	153	52.917	-0.157	35.168	1.00	53.73	C
ATOM	1065	CB	ALA	A	153	52.169	1.169	35.102	1.00	56.83	C
ATOM	1066	C	ALA	A	153	54.351	0.090	35.604	1.00	53.75	C
ATOM	1067	O	ALA	A	153	55.162	0.555	34.806	1.00	50.96	O
ATOM	1068	N	ASN	A	154	54.663	-0.224	36.864	1.00	54.77	N
ATOM	1069	CA	ASN	A	154	56.010	-0.002	37.401	1.00	55.40	C
ATOM	1070	CB	ASN	A	154	55.964	1.138	38.411	1.00	56.32	C
ATOM	1071	CG	ASN	A	154	55.429	2.412	37.810	1.00	60.48	C
ATOM	1072	OD1	ASN	A	154	54.883	3.262	38.511	1.00	65.32	O
ATOM	1073	ND2	ASN	A	154	55.588	2.558	36.500	1.00	62.17	N
ATOM	1074	C	ASN	A	154	56.717	-1.213	38.029	1.00	55.61	C
ATOM	1075	O	ASN	A	154	57.810	-1.579	37.602	1.00	57.04	O
ATOM	1076	N	SER	A	155	56.116	-1.820	39.045	1.00	53.92	N
ATOM	1077	CA	SER	A	155	56.730	-2.972	39.688	1.00	53.22	C
ATOM	1078	CB	SER	A	155	55.666	-3.877	40.318	1.00	53.29	C
ATOM	1079	OG	SER	A	155	56.187	-5.164	40.632	1.00	47.63	O
ATOM	1080	C	SER	A	155	57.532	-3.798	38.699	1.00	55.53	C
ATOM	1081	O	SER	A	155	57.150	-3.944	37.535	1.00	51.70	O
ATOM	1082	N	LEU	A	156	58.658	-4.319	39.181	1.00	59.63	N
ATOM	1083	CA	LEU	A	156	59.536	-5.184	38.396	1.00	58.25	C
ATOM	1084	CB	LEU	A	156	60.948	-4.589	38.298	1.00	53.27	C
ATOM	1085	CG	LEU	A	156	60.959	-3.198	37.656	1.00	52.46	C
ATOM	1086	CD1	LEU	A	156	60.724	-2.160	38.748	1.00	54.13	C
ATOM	1087	CD2	LEU	A	156	62.265	-2.924	36.939	1.00	45.69	C
ATOM	1088	C	LEU	A	156	59.553	-6.536	39.116	1.00	57.39	C
ATOM	1089	O	LEU	A	156	60.114	-7.510	38.645	1.00	58.31	O
ATOM	1090	N	ASP	A	157	58.897	-6.595	40.259	1.00	56.37	N
ATOM	1091	CA	ASP	A	157	58.861	-7.831	40.990	1.00	59.57	C
ATOM	1092	CB	ASP	A	157	58.439	-7.573	42.432	1.00	67.57	C
ATOM	1093	CG	ASP	A	157	58.602	-8.802	43.309	1.00	75.23	C
ATOM	1094	OD1	ASP	A	157	59.757	-9.260	43.500	1.00	78.50	O
ATOM	1095	OD2	ASP	A	157	57.572	-9.314	43.799	1.00	78.19	O
ATOM	1096	C	ASP	A	157	57.889	-8.803	40.350	1.00	57.71	C
ATOM	1097	O	ASP	A	157	56.695	-8.740	40.621	1.00	60.50	O
ATOM	1098	N	TYR	A	158	58.390	-9.699	39.507	1.00	54.14	N
ATOM	1099	CA	TYR	A	158	57.545	-10.706	38.849	1.00	53.93	C
ATOM	1100	CB	TYR	A	158	58.385	-11.927	38.494	1.00	46.09	C
ATOM	1101	CG	TYR	A	158	57.645	-13.028	37.790	1.00	42.52	C
ATOM	1102	CD1	TYR	A	158	57.701	-13.150	36.406	1.00	45.48	C
ATOM	1103	CE1	TYR	A	158	56.998	-14.149	35.732	1.00	43.70	C
ATOM	1104	CD2	TYR	A	158	56.870	-13.939	38.497	1.00	43.48	C
ATOM	1105	CE2	TYR	A	158	56.160	-14.948	37.835	1.00	45.09	C
ATOM	1106	CZ	TYR	A	158	56.226	-15.041	36.450	1.00	46.22	C
ATOM	1107	OH	TYR	A	158	55.484	-15.984	35.773	1.00	46.66	O
ATOM	1108	C	TYR	A	158	56.387	-11.161	39.744	1.00	58.48	C
ATOM	1109	O	TYR	A	158	55.350	-11.614	39.261	1.00	60.79	O
ATOM	1110	N	ASN	A	159	56.575	-11.040	41.053	1.00	61.86	N
ATOM	1111	CA	ASN	A	159	55.572	-11.457	42.023	1.00	65.08	C
ATOM	1112	CB	ASN	A	159	56.274	-11.955	43.298	1.00	67.08	C
ATOM	1113	CG	ASN	A	159	57.066	-13.235	43.063	1.00	66.68	C
ATOM	1114	OD1	ASN	A	159	56.493	-14.324	42.994	1.00	64.52	O
ATOM	1115	ND2	ASN	A	159	58.385	-13.105	42.918	1.00	64.23	N
ATOM	1116	C	ASN	A	159	54.556	-10.370	42.351	1.00	65.71	C
ATOM	1117	O	ASN	A	159	53.366	-10.654	42.476	1.00	67.38	O
ATOM	1118	N	GLU	A	160	55.019	-9.134	42.516	1.00	66.66	N

310/396

Figure 3B-21

ATOM	1119	CA	GLU	A	160	54.110	-8.017	42.787	1.00	64.77	C
ATOM	1120	CB	GLU	A	160	54.895	-6.707	42.928	1.00	64.13	C
ATOM	1121	CG	GLU	A	160	54.086	-5.499	43.372	1.00	62.49	C
ATOM	1122	CD	GLU	A	160	54.957	-4.250	43.550	1.00	67.91	C
ATOM	1123	OE1	GLU	A	160	54.447	-3.226	44.046	1.00	71.30	O
ATOM	1124	OE2	GLU	A	160	56.157	-4.281	43.196	1.00	67.49	O
ATOM	1125	C	GLU	A	160	53.255	-7.980	41.525	1.00	64.45	C
ATOM	1126	O	GLU	A	160	52.028	-8.071	41.586	1.00	64.76	O
ATOM	1127	N	ARG	A	161	53.926	-7.874	40.379	1.00	60.03	N
ATOM	1128	CA	ARG	A	161	53.246	-7.855	39.104	1.00	56.54	C
ATOM	1129	CB	ARG	A	161	54.207	-8.177	37.961	1.00	54.38	C
ATOM	1130	CG	ARG	A	161	55.386	-7.252	37.819	1.00	56.51	C
ATOM	1131	CD	ARG	A	161	54.959	-5.823	37.586	1.00	57.91	C
ATOM	1132	NE	ARG	A	161	54.161	-5.664	36.376	1.00	57.64	N
ATOM	1133	CZ	ARG	A	161	54.654	-5.559	35.152	1.00	54.51	C
ATOM	1134	NH1	ARG	A	161	55.959	-5.590	34.948	1.00	58.04	N
ATOM	1135	NH2	ARG	A	161	53.831	-5.419	34.131	1.00	55.86	N
ATOM	1136	C	ARG	A	161	52.193	-8.941	39.143	1.00	56.37	C
ATOM	1137	O	ARG	A	161	51.006	-8.687	38.979	1.00	60.37	O
ATOM	1138	N	LEU	A	162	52.642	-10.160	39.390	1.00	54.79	N
ATOM	1139	CA	LEU	A	162	51.760	-11.317	39.408	1.00	53.49	C
ATOM	1140	CB	LEU	A	162	52.576	-12.552	39.737	1.00	50.73	C
ATOM	1141	CG	LEU	A	162	52.139	-13.733	38.897	1.00	47.88	C
ATOM	1142	CD1	LEU	A	162	53.233	-14.754	38.933	1.00	50.84	C
ATOM	1143	CD2	LEU	A	162	50.819	-14.288	39.399	1.00	42.65	C
ATOM	1144	C	LEU	A	162	50.526	-11.259	40.302	1.00	53.26	C
ATOM	1145	O	LEU	A	162	49.428	-11.595	39.864	1.00	51.32	O
ATOM	1146	N	TRP	A	163	50.698	-10.858	41.557	1.00	57.00	N
ATOM	1147	CA	TRP	A	163	49.560	-10.771	42.469	1.00	58.67	C
ATOM	1148	CB	TRP	A	163	50.018	-10.260	43.851	1.00	60.05	C
ATOM	1149	CG	TRP	A	163	48.878	-9.884	44.763	1.00	64.16	C
ATOM	1150	CD2	TRP	A	163	48.421	-8.555	45.044	1.00	65.84	C
ATOM	1151	CE2	TRP	A	163	47.251	-8.669	45.823	1.00	64.33	C
ATOM	1152	CE3	TRP	A	163	48.888	-7.280	44.704	1.00	65.13	C
ATOM	1153	CD1	TRP	A	163	47.992	-10.730	45.383	1.00	63.61	C
ATOM	1154	NE1	TRP	A	163	47.009	-10.003	46.018	1.00	62.49	N
ATOM	1155	CZ2	TRP	A	163	46.546	-7.559	46.260	1.00	66.08	C
ATOM	1156	CZ3	TRP	A	163	48.185	-6.182	45.140	1.00	63.87	C
ATOM	1157	CH2	TRP	A	163	47.027	-6.325	45.908	1.00	65.81	C
ATOM	1158	C	TRP	A	163	48.526	-9.829	41.840	1.00	57.34	C
ATOM	1159	O	TRP	A	163	47.431	-10.255	41.456	1.00	51.82	O
ATOM	1160	N	ALA	A	164	48.904	-8.556	41.721	1.00	58.56	N
ATOM	1161	CA	ALA	A	164	48.055	-7.519	41.124	1.00	60.02	C
ATOM	1162	CB	ALA	A	164	48.924	-6.363	40.599	1.00	59.08	C
ATOM	1163	C	ALA	A	164	47.217	-8.083	39.987	1.00	59.11	C
ATOM	1164	O	ALA	A	164	45.990	-8.056	40.040	1.00	59.78	O
ATOM	1165	N	TRP	A	165	47.904	-8.581	38.964	1.00	56.65	N
ATOM	1166	CA	TRP	A	165	47.284	-9.171	37.789	1.00	57.68	C
ATOM	1167	CB	TRP	A	165	48.360	-9.837	36.949	1.00	57.49	C
ATOM	1168	CG	TRP	A	165	47.903	-10.302	35.613	1.00	56.79	C
ATOM	1169	CD2	TRP	A	165	47.185	-11.506	35.311	1.00	53.78	C
ATOM	1170	CE2	TRP	A	165	47.002	-11.542	33.917	1.00	56.29	C
ATOM	1171	CE3	TRP	A	165	46.681	-12.551	36.081	1.00	52.35	C
ATOM	1172	CD1	TRP	A	165	48.115	-9.677	34.429	1.00	58.68	C
ATOM	1173	NE1	TRP	A	165	47.580	-10.415	33.402	1.00	61.12	N
ATOM	1174	CZ2	TRP	A	165	46.335	-12.582	33.275	1.00	52.94	C

311/396

Figure 3B-22

ATOM	1175	CZ3	TRP	A	165	46.020	-13.580	35.443	1.00	52.74	C
ATOM	1176	CH2	TRP	A	165	45.853	-13.587	34.053	1.00	52.32	C
ATOM	1177	C	TRP	A	165	46.209	-10.208	38.123	1.00	60.10	C
ATOM	1178	O	TRP	A	165	45.061	-10.085	37.708	1.00	62.12	O
ATOM	1179	N	GLU	A	166	46.591	-11.242	38.860	1.00	60.81	N
ATOM	1180	CA	GLU	A	166	45.661	-12.306	39.221	1.00	60.97	C
ATOM	1181	CB	GLU	A	166	46.462	-13.470	39.842	1.00	59.51	C
ATOM	1182	CG	GLU	A	166	45.645	-14.610	40.478	1.00	59.40	C
ATOM	1183	CD	GLU	A	166	44.703	-15.311	39.509	1.00	58.79	C
ATOM	1184	OE1	GLU	A	166	45.076	-15.459	38.330	1.00	63.39	O
ATOM	1185	OE2	GLU	A	166	43.601	-15.729	39.924	1.00	52.96	O
ATOM	1186	C	GLU	A	166	44.538	-11.825	40.160	1.00	61.06	C
ATOM	1187	O	GLU	A	166	43.344	-12.003	39.878	1.00	56.62	O
ATOM	1188	N	SER	A	167	44.928	-11.214	41.273	1.00	62.58	N
ATOM	1189	CA	SER	A	167	43.968	-10.716	42.251	1.00	62.07	C
ATOM	1190	CB	SER	A	167	44.680	-9.824	43.282	1.00	63.76	C
ATOM	1191	OG	SER	A	167	45.618	-8.948	42.673	1.00	62.55	O
ATOM	1192	C	SER	A	167	42.840	-9.953	41.570	1.00	60.33	C
ATOM	1193	O	SER	A	167	41.687	-10.340	41.663	1.00	59.69	O
ATOM	1194	N	TRP	A	168	43.187	-8.873	40.880	1.00	58.79	N
ATOM	1195	CA	TRP	A	168	42.213	-8.059	40.174	1.00	56.32	C
ATOM	1196	CB	TRP	A	168	42.923	-7.109	39.210	1.00	54.09	C
ATOM	1197	CG	TRP	A	168	41.986	-6.326	38.352	1.00	53.22	C
ATOM	1198	CD2	TRP	A	168	41.002	-5.377	38.787	1.00	51.75	C
ATOM	1199	CE2	TRP	A	168	40.363	-4.881	37.638	1.00	49.29	C
ATOM	1200	CE3	TRP	A	168	40.600	-4.901	40.039	1.00	51.97	C
ATOM	1201	CD1	TRP	A	168	41.901	-6.363	36.996	1.00	54.10	C
ATOM	1202	NE1	TRP	A	168	40.930	-5.498	36.557	1.00	51.19	N
ATOM	1203	CZ2	TRP	A	168	39.353	-3.936	37.696	1.00	49.96	C
ATOM	1204	CZ3	TRP	A	168	39.590	-3.959	40.097	1.00	51.19	C
ATOM	1205	CH2	TRP	A	168	38.980	-3.488	38.934	1.00	52.59	C
ATOM	1206	C	TRP	A	168	41.230	-8.930	39.406	1.00	57.06	C
ATOM	1207	O	TRP	A	168	40.030	-8.873	39.655	1.00	59.68	O
ATOM	1208	N	ARG	A	169	41.736	-9.738	38.476	1.00	56.89	N
ATOM	1209	CA	ARG	A	169	40.876	-10.620	37.686	1.00	56.65	C
ATOM	1210	CB	ARG	A	169	41.705	-11.415	36.654	1.00	54.80	C
ATOM	1211	CG	ARG	A	169	42.191	-10.576	35.457	1.00	54.21	C
ATOM	1212	CD	ARG	A	169	43.073	-11.364	34.494	1.00	51.35	C
ATOM	1213	NE	ARG	A	169	43.587	-10.555	33.383	1.00	52.10	N
ATOM	1214	CZ	ARG	A	169	44.264	-9.410	33.513	1.00	53.41	C
ATOM	1215	NH1	ARG	A	169	44.696	-8.759	32.439	1.00	47.10	N
ATOM	1216	NH2	ARG	A	169	44.507	-8.899	34.713	1.00	52.72	N
ATOM	1217	C	ARG	A	169	40.111	-11.581	38.594	1.00	58.94	C
ATOM	1218	O	ARG	A	169	38.939	-11.883	38.346	1.00	58.13	O
ATOM	1219	N	SER	A	170	40.779	-12.045	39.652	1.00	59.86	N
ATOM	1220	CA	SER	A	170	40.188	-12.977	40.608	1.00	58.70	C
ATOM	1221	CB	SER	A	170	41.271	-13.566	41.489	1.00	59.74	C
ATOM	1222	OG	SER	A	170	40.675	-14.257	42.567	1.00	63.55	O
ATOM	1223	C	SER	A	170	39.124	-12.358	41.500	1.00	59.38	C
ATOM	1224	O	SER	A	170	38.012	-12.860	41.596	1.00	59.79	O
ATOM	1225	N	GLU	A	171	39.474	-11.276	42.179	1.00	61.70	N
ATOM	1226	CA	GLU	A	171	38.516	-10.616	43.045	1.00	63.29	C
ATOM	1227	CB	GLU	A	171	39.187	-9.545	43.921	1.00	68.35	C
ATOM	1228	CG	GLU	A	171	39.360	-9.953	45.397	1.00	71.85	C
ATOM	1229	CD	GLU	A	171	40.672	-10.686	45.672	1.00	74.77	C
ATOM	1230	OE1	GLU	A	171	41.731	-10.018	45.712	1.00	76.12	O

312/396

Figure 3B-23

ATOM	1231	OE2	GLU	A	171	40.647	-11.926	45.846	1.00	74.30	O
ATOM	1232	C	GLU	A	171	37.399	-9.994	42.226	1.00	61.66	C
ATOM	1233	O	GLU	A	171	36.264	-10.456	42.303	1.00	64.27	O
ATOM	1234	N	VAL	A	172	37.699	-8.968	41.432	1.00	57.11	N
ATOM	1235	CA	VAL	A	172	36.644	-8.343	40.648	1.00	55.45	C
ATOM	1236	CB	VAL	A	172	37.021	-6.924	40.195	1.00	55.14	C
ATOM	1237	CG1	VAL	A	172	37.374	-6.081	41.402	1.00	59.27	C
ATOM	1238	CG2	VAL	A	172	38.155	-6.966	39.213	1.00	53.26	C
ATOM	1239	C	VAL	A	172	36.208	-9.135	39.427	1.00	54.57	C
ATOM	1240	O	VAL	A	172	35.036	-9.471	39.292	1.00	53.26	O
ATOM	1241	N	GLY	A	173	37.142	-9.442	38.539	1.00	55.11	N
ATOM	1242	CA	GLY	A	173	36.787	-10.175	37.340	1.00	57.20	C
ATOM	1243	C	GLY	A	173	35.672	-11.185	37.539	1.00	59.78	C
ATOM	1244	O	GLY	A	173	34.704	-11.219	36.777	1.00	59.88	O
ATOM	1245	N	LYS	A	174	35.819	-12.006	38.573	1.00	61.36	N
ATOM	1246	CA	LYS	A	174	34.855	-13.045	38.905	1.00	62.04	C
ATOM	1247	CB	LYS	A	174	35.253	-13.716	40.212	1.00	65.08	C
ATOM	1248	CG	LYS	A	174	35.728	-15.139	40.072	1.00	68.56	C
ATOM	1249	CD	LYS	A	174	36.991	-15.240	39.257	1.00	72.77	C
ATOM	1250	CE	LYS	A	174	37.906	-16.299	39.859	1.00	77.45	C
ATOM	1251	NZ	LYS	A	174	37.167	-17.528	40.274	1.00	76.46	N
ATOM	1252	C	LYS	A	174	33.447	-12.505	39.042	1.00	62.52	C
ATOM	1253	O	LYS	A	174	32.501	-13.045	38.468	1.00	65.91	O
ATOM	1254	N	GLN	A	175	33.310	-11.443	39.824	1.00	61.06	N
ATOM	1255	CA	GLN	A	175	32.012	-10.829	40.046	1.00	60.38	C
ATOM	1256	CB	GLN	A	175	32.164	-9.536	40.846	1.00	62.91	C
ATOM	1257	CG	GLN	A	175	32.767	-9.686	42.232	1.00	61.49	C
ATOM	1258	CD	GLN	A	175	32.649	-8.408	43.033	1.00	63.63	C
ATOM	1259	OE1	GLN	A	175	31.548	-7.861	43.199	1.00	61.95	O
ATOM	1260	NE2	GLN	A	175	33.780	-7.920	43.534	1.00	64.88	N
ATOM	1261	C	GLN	A	175	31.360	-10.502	38.718	1.00	59.83	C
ATOM	1262	O	GLN	A	175	30.181	-10.774	38.509	1.00	58.58	O
ATOM	1263	N	LEU	A	176	32.144	-9.899	37.830	1.00	59.25	N
ATOM	1264	CA	LEU	A	176	31.661	-9.519	36.515	1.00	59.87	C
ATOM	1265	CB	LEU	A	176	32.800	-8.950	35.657	1.00	55.67	C
ATOM	1266	CG	LEU	A	176	33.319	-7.532	35.892	1.00	48.86	C
ATOM	1267	CD1	LEU	A	176	32.155	-6.571	36.089	1.00	43.17	C
ATOM	1268	CD2	LEU	A	176	34.220	-7.533	37.083	1.00	48.57	C
ATOM	1269	C	LEU	A	176	31.026	-10.689	35.773	1.00	63.00	C
ATOM	1270	O	LEU	A	176	29.900	-10.582	35.281	1.00	67.51	O
ATOM	1271	N	ARG	A	177	31.744	-11.805	35.695	1.00	61.76	N
ATOM	1272	CA	ARG	A	177	31.250	-12.971	34.981	1.00	61.22	C
ATOM	1273	CB	ARG	A	177	31.913	-14.238	35.530	1.00	61.86	C
ATOM	1274	CG	ARG	A	177	31.655	-15.461	34.672	1.00	63.24	C
ATOM	1275	CD	ARG	A	177	31.892	-15.124	33.213	1.00	61.90	C
ATOM	1276	NE	ARG	A	177	31.574	-16.229	32.318	1.00	62.66	N
ATOM	1277	CZ	ARG	A	177	32.413	-17.209	32.007	1.00	64.16	C
ATOM	1278	NH1	ARG	A	177	32.025	-18.169	31.179	1.00	64.82	N
ATOM	1279	NH2	ARG	A	177	33.639	-17.228	32.511	1.00	63.12	N
ATOM	1280	C	ARG	A	177	29.721	-13.131	34.940	1.00	60.62	C
ATOM	1281	O	ARG	A	177	29.097	-12.815	33.931	1.00	58.24	O
ATOM	1282	N	PRO	A	178	29.098	-13.576	36.046	1.00	61.95	N
ATOM	1283	CD	PRO	A	178	29.682	-13.592	37.399	1.00	62.09	C
ATOM	1284	CA	PRO	A	178	27.643	-13.781	36.126	1.00	62.34	C
ATOM	1285	CB	PRO	A	178	27.360	-13.685	37.619	1.00	60.72	C
ATOM	1286	CG	PRO	A	178	28.585	-14.259	38.212	1.00	62.92	C

313/396

Figure 3B-24

ATOM	1287	C	PRO	A	178	26.807	-12.791	35.348	1.00	63.11	C
ATOM	1288	O	PRO	A	178	25.868	-13.165	34.651	1.00	64.89	O
ATOM	1289	N	LEU	A	179	27.145	-11.519	35.483	1.00	64.89	N
ATOM	1290	CA	LEU	A	179	26.402	-10.473	34.804	1.00	65.70	C
ATOM	1291	CB	LEU	A	179	26.566	-9.130	35.531	1.00	65.65	C
ATOM	1292	CG	LEU	A	179	26.009	-8.987	36.950	1.00	63.55	C
ATOM	1293	CD1	LEU	A	179	26.077	-7.531	37.333	1.00	60.60	C
ATOM	1294	CD2	LEU	A	179	24.561	-9.485	37.030	1.00	62.08	C
ATOM	1295	C	LEU	A	179	26.814	-10.312	33.354	1.00	65.16	C
ATOM	1296	O	LEU	A	179	26.035	-9.807	32.549	1.00	66.72	O
ATOM	1297	N	TYR	A	180	28.030	-10.720	33.008	1.00	63.33	N
ATOM	1298	CA	TYR	A	180	28.442	-10.567	31.624	1.00	64.26	C
ATOM	1299	CB	TYR	A	180	29.934	-10.815	31.436	1.00	62.90	C
ATOM	1300	CG	TYR	A	180	30.438	-10.221	30.141	1.00	61.85	C
ATOM	1301	CD1	TYR	A	180	30.444	-8.848	29.947	1.00	61.24	C
ATOM	1302	CE1	TYR	A	180	30.844	-8.290	28.742	1.00	62.45	C
ATOM	1303	CD2	TYR	A	180	30.850	-11.028	29.092	1.00	63.72	C
ATOM	1304	CE2	TYR	A	180	31.250	-10.478	27.873	1.00	63.49	C
ATOM	1305	CZ	TYR	A	180	31.245	-9.108	27.708	1.00	62.09	C
ATOM	1306	OH	TYR	A	180	31.655	-8.553	26.518	1.00	57.58	O
ATOM	1307	C	TYR	A	180	27.659	-11.569	30.816	1.00	65.26	C
ATOM	1308	O	TYR	A	180	27.175	-11.272	29.728	1.00	66.15	O
ATOM	1309	N	GLU	A	181	27.526	-12.765	31.366	1.00	66.91	N
ATOM	1310	CA	GLU	A	181	26.781	-13.804	30.690	1.00	66.69	C
ATOM	1311	CB	GLU	A	181	26.716	-15.057	31.576	1.00	63.54	C
ATOM	1312	CG	GLU	A	181	28.100	-15.445	32.121	1.00	63.92	C
ATOM	1313	CD	GLU	A	181	28.240	-16.908	32.539	1.00	64.27	C
ATOM	1314	OE1	GLU	A	181	27.352	-17.415	33.256	1.00	65.03	O
ATOM	1315	OE2	GLU	A	181	29.256	-17.546	32.160	1.00	57.79	O
ATOM	1316	C	GLU	A	181	25.394	-13.247	30.357	1.00	67.05	C
ATOM	1317	O	GLU	A	181	24.929	-13.386	29.232	1.00	67.38	O
ATOM	1318	N	GLU	A	182	24.749	-12.581	31.310	1.00	67.61	N
ATOM	1319	CA	GLU	A	182	23.421	-12.014	31.052	1.00	70.11	C
ATOM	1320	CB	GLU	A	182	22.789	-11.481	32.338	1.00	71.80	C
ATOM	1321	CG	GLU	A	182	22.660	-12.492	33.458	1.00	78.77	C
ATOM	1322	CD	GLU	A	182	22.038	-11.885	34.709	1.00	81.96	C
ATOM	1323	OE1	GLU	A	182	20.915	-11.335	34.606	1.00	82.63	O
ATOM	1324	OE2	GLU	A	182	22.669	-11.957	35.788	1.00	81.81	O
ATOM	1325	C	GLU	A	182	23.492	-10.866	30.052	1.00	69.23	C
ATOM	1326	O	GLU	A	182	22.593	-10.678	29.237	1.00	70.17	O
ATOM	1327	N	TYR	A	183	24.566	-10.094	30.128	1.00	67.46	N
ATOM	1328	CA	TYR	A	183	24.743	-8.948	29.251	1.00	64.45	C
ATOM	1329	CB	TYR	A	183	26.032	-8.198	29.655	1.00	58.30	C
ATOM	1330	CG	TYR	A	183	26.643	-7.310	28.592	1.00	53.58	C
ATOM	1331	CD1	TYR	A	183	27.799	-7.693	27.932	1.00	52.32	C
ATOM	1332	CE1	TYR	A	183	28.371	-6.894	26.963	1.00	50.43	C
ATOM	1333	CD2	TYR	A	183	26.070	-6.096	28.247	1.00	51.41	C
ATOM	1334	CE2	TYR	A	183	26.638	-5.289	27.271	1.00	48.57	C
ATOM	1335	CZ	TYR	A	183	27.790	-5.695	26.637	1.00	48.68	C
ATOM	1336	OH	TYR	A	183	28.383	-4.896	25.686	1.00	47.91	O
ATOM	1337	C	TYR	A	183	24.732	-9.341	27.770	1.00	64.16	C
ATOM	1338	O	TYR	A	183	23.993	-8.751	26.980	1.00	62.03	O
ATOM	1339	N	VAL	A	184	25.520	-10.345	27.394	1.00	64.69	N
ATOM	1340	CA	VAL	A	184	25.555	-10.756	25.993	1.00	67.55	C
ATOM	1341	CB	VAL	A	184	26.580	-11.923	25.730	1.00	67.88	C
ATOM	1342	CG1	VAL	A	184	27.780	-11.798	26.656	1.00	65.33	C

314/396

Figure 3B-25

ATOM	1343	CG2	VAL	A	184	25.904	-13.280	25.879	1.00	69.33	C
ATOM	1344	C	VAL	A	184	24.152	-11.197	25.560	1.00	68.75	C
ATOM	1345	O	VAL	A	184	23.664	-10.782	24.510	1.00	69.42	O
ATOM	1346	N	VAL	A	185	23.503	-12.020	26.380	1.00	68.02	N
ATOM	1347	CA	VAL	A	185	22.159	-12.507	26.097	1.00	67.71	C
ATOM	1348	CB	VAL	A	185	21.630	-13.351	27.259	1.00	67.90	C
ATOM	1349	CG1	VAL	A	185	20.230	-13.838	26.944	1.00	67.98	C
ATOM	1350	CG2	VAL	A	185	22.568	-14.513	27.521	1.00	68.05	C
ATOM	1351	C	VAL	A	185	21.177	-11.362	25.870	1.00	69.01	C
ATOM	1352	O	VAL	A	185	20.577	-11.244	24.805	1.00	69.61	O
ATOM	1353	N	LEU	A	186	21.006	-10.520	26.881	1.00	70.23	N
ATOM	1354	CA	LEU	A	186	20.093	-9.390	26.769	1.00	71.81	C
ATOM	1355	CB	LEU	A	186	20.121	-8.549	28.044	1.00	69.88	C
ATOM	1356	CG	LEU	A	186	19.297	-9.061	29.220	1.00	68.79	C
ATOM	1357	CD1	LEU	A	186	17.884	-9.329	28.717	1.00	67.48	C
ATOM	1358	CD2	LEU	A	186	19.920	-10.317	29.815	1.00	67.72	C
ATOM	1359	C	LEU	A	186	20.429	-8.495	25.587	1.00	72.75	C
ATOM	1360	O	LEU	A	186	19.572	-8.165	24.772	1.00	72.29	O
ATOM	1361	N	LYS	A	187	21.688	-8.098	25.508	1.00	74.48	N
ATOM	1362	CA	LYS	A	187	22.135	-7.221	24.445	1.00	75.94	C
ATOM	1363	CB	LYS	A	187	23.632	-6.934	24.633	1.00	78.00	C
ATOM	1364	CG	LYS	A	187	24.084	-5.506	24.307	1.00	78.91	C
ATOM	1365	CD	LYS	A	187	23.499	-4.477	25.265	1.00	77.93	C
ATOM	1366	CE	LYS	A	187	24.033	-3.091	24.951	1.00	78.14	C
ATOM	1367	NZ	LYS	A	187	23.354	-2.030	25.741	1.00	79.30	N
ATOM	1368	C	LYS	A	187	21.855	-7.862	23.077	1.00	76.16	C
ATOM	1369	O	LYS	A	187	21.459	-7.175	22.132	1.00	74.06	O
ATOM	1370	N	ASN	A	188	22.050	-9.178	22.988	1.00	77.22	N
ATOM	1371	CA	ASN	A	188	21.832	-9.931	21.746	1.00	78.23	C
ATOM	1372	CB	ASN	A	188	22.177	-11.407	21.961	1.00	74.29	C
ATOM	1373	CG	ASN	A	188	23.369	-11.855	21.149	1.00	70.72	C
ATOM	1374	OD1	ASN	A	188	24.227	-11.056	20.785	1.00	70.46	O
ATOM	1375	ND2	ASN	A	188	23.438	-13.148	20.875	1.00	71.02	N
ATOM	1376	C	ASN	A	188	20.383	-9.806	21.296	1.00	80.50	C
ATOM	1377	O	ASN	A	188	20.105	-9.388	20.171	1.00	80.29	O
ATOM	1378	N	GLU	A	189	19.469	-10.178	22.185	1.00	82.06	N
ATOM	1379	CA	GLU	A	189	18.044	-10.093	21.908	1.00	85.29	C
ATOM	1380	CB	GLU	A	189	17.253	-10.322	23.199	1.00	86.30	C
ATOM	1381	CG	GLU	A	189	15.747	-10.422	23.006	1.00	89.08	C
ATOM	1382	CD	GLU	A	189	15.015	-10.742	24.296	1.00	90.15	C
ATOM	1383	OE1	GLU	A	189	15.509	-11.605	25.051	1.00	90.98	O
ATOM	1384	OE2	GLU	A	189	13.944	-10.144	24.551	1.00	91.34	O
ATOM	1385	C	GLU	A	189	17.722	-8.711	21.341	1.00	86.59	C
ATOM	1386	O	GLU	A	189	17.038	-8.586	20.333	1.00	87.81	O
ATOM	1387	N	MET	A	190	18.221	-7.674	22.001	1.00	88.76	N
ATOM	1388	CA	MET	A	190	17.996	-6.303	21.560	1.00	89.64	C
ATOM	1389	CB	MET	A	190	18.690	-5.326	22.525	1.00	91.55	C
ATOM	1390	CG	MET	A	190	18.765	-3.880	22.044	1.00	95.08	C
ATOM	1391	SD	MET	A	190	20.238	-3.480	21.050	1.00	101.13	S
ATOM	1392	CE	MET	A	190	21.094	-2.303	22.135	1.00	101.02	C
ATOM	1393	C	MET	A	190	18.532	-6.126	20.145	1.00	88.80	C
ATOM	1394	O	MET	A	190	17.879	-5.529	19.293	1.00	88.92	O
ATOM	1395	N	ALA	A	191	19.721	-6.663	19.899	1.00	87.78	N
ATOM	1396	CA	ALA	A	191	20.351	-6.555	18.591	1.00	87.44	C
ATOM	1397	CB	ALA	A	191	21.758	-7.132	18.637	1.00	87.48	C
ATOM	1398	C	ALA	A	191	19.552	-7.265	17.518	1.00	87.23	C

315/396

Figure 3B-26

ATOM	1399	O	ALA	A	191	18.893	-6.631	16.695	1.00	86.89	O
ATOM	1400	N	ARG	A	192	19.629	-8.592	17.538	1.00	86.27	N
ATOM	1401	CA	ARG	A	192	18.952	-9.431	16.563	1.00	84.00	C
ATOM	1402	CB	ARG	A	192	19.108	-10.902	16.959	1.00	82.21	C
ATOM	1403	CG	ARG	A	192	20.573	-11.344	17.013	1.00	83.43	C
ATOM	1404	CD	ARG	A	192	20.728	-12.766	17.494	1.00	81.81	C
ATOM	1405	NE	ARG	A	192	19.770	-13.039	18.558	1.00	86.07	N
ATOM	1406	CZ	ARG	A	192	19.806	-14.101	19.354	1.00	87.20	C
ATOM	1407	NH1	ARG	A	192	18.875	-14.253	20.287	1.00	87.15	N
ATOM	1408	NH2	ARG	A	192	20.778	-14.999	19.231	1.00	87.88	N
ATOM	1409	C	ARG	A	192	17.488	-9.072	16.359	1.00	83.48	C
ATOM	1410	O	ARG	A	192	16.952	-9.258	15.272	1.00	86.04	O
ATOM	1411	N	ALA	A	193	16.836	-8.546	17.388	1.00	82.45	N
ATOM	1412	CA	ALA	A	193	15.437	-8.167	17.254	1.00	80.86	C
ATOM	1413	CB	ALA	A	193	14.762	-8.143	18.613	1.00	80.30	C
ATOM	1414	C	ALA	A	193	15.369	-6.794	16.603	1.00	81.21	C
ATOM	1415	O	ALA	A	193	14.315	-6.158	16.562	1.00	81.55	O
ATOM	1416	N	ASN	A	194	16.512	-6.335	16.101	1.00	81.87	N
ATOM	1417	CA	ASN	A	194	16.590	-5.042	15.431	1.00	81.70	C
ATOM	1418	CB	ASN	A	194	17.482	-4.068	16.208	1.00	81.53	C
ATOM	1419	CG	ASN	A	194	16.700	-2.894	16.768	1.00	81.43	C
ATOM	1420	OD1	ASN	A	194	15.985	-2.204	16.034	1.00	79.44	O
ATOM	1421	ND2	ASN	A	194	16.828	-2.662	18.073	1.00	81.25	N
ATOM	1422	C	ASN	A	194	17.102	-5.208	14.007	1.00	80.14	C
ATOM	1423	O	ASN	A	194	17.615	-4.267	13.398	1.00	78.43	O
ATOM	1424	N	HIS	A	195	16.956	-6.426	13.493	1.00	78.82	N
ATOM	1425	CA	HIS	A	195	17.341	-6.748	12.132	1.00	76.51	C
ATOM	1426	CB	HIS	A	195	16.805	-5.669	11.189	1.00	78.96	C
ATOM	1427	CG	HIS	A	195	15.342	-5.392	11.371	1.00	83.30	C
ATOM	1428	CD2	HIS	A	195	14.326	-6.194	11.774	1.00	82.71	C
ATOM	1429	ND1	HIS	A	195	14.784	-4.149	11.154	1.00	84.19	N
ATOM	1430	CE1	HIS	A	195	13.489	-4.196	11.421	1.00	83.72	C
ATOM	1431	NE2	HIS	A	195	13.187	-5.426	11.798	1.00	83.03	N
ATOM	1432	C	HIS	A	195	18.833	-6.910	11.948	1.00	74.30	C
ATOM	1433	O	HIS	A	195	19.354	-6.654	10.864	1.00	76.36	O
ATOM	1434	N	TYR	A	196	19.524	-7.326	13.006	1.00	70.66	N
ATOM	1435	CA	TYR	A	196	20.967	-7.544	12.931	1.00	67.08	C
ATOM	1436	CB	TYR	A	196	21.731	-6.589	13.861	1.00	66.55	C
ATOM	1437	CG	TYR	A	196	21.807	-5.136	13.404	1.00	64.43	C
ATOM	1438	CD1	TYR	A	196	22.646	-4.744	12.359	1.00	63.82	C
ATOM	1439	CE1	TYR	A	196	22.720	-3.404	11.958	1.00	62.84	C
ATOM	1440	CD2	TYR	A	196	21.047	-4.154	14.030	1.00	61.81	C
ATOM	1441	CE2	TYR	A	196	21.112	-2.825	13.635	1.00	59.81	C
ATOM	1442	CZ	TYR	A	196	21.944	-2.454	12.606	1.00	61.54	C
ATOM	1443	OH	TYR	A	196	21.988	-1.126	12.240	1.00	62.43	O
ATOM	1444	C	TYR	A	196	21.216	-8.980	13.343	1.00	65.14	C
ATOM	1445	O	TYR	A	196	20.381	-9.593	13.992	1.00	60.25	O
ATOM	1446	N	GLU	A	197	22.371	-9.508	12.963	1.00	68.11	N
ATOM	1447	CA	GLU	A	197	22.732	-10.891	13.260	1.00	71.26	C
ATOM	1448	CB	GLU	A	197	23.907	-11.297	12.381	1.00	71.47	C
ATOM	1449	CG	GLU	A	197	23.582	-11.146	10.911	1.00	72.88	C
ATOM	1450	CD	GLU	A	197	24.803	-11.123	10.038	1.00	74.45	C
ATOM	1451	OE1	GLU	A	197	25.632	-12.062	10.158	1.00	74.06	O
ATOM	1452	OE2	GLU	A	197	24.920	-10.164	9.236	1.00	71.20	O
ATOM	1453	C	GLU	A	197	23.071	-11.111	14.717	1.00	72.03	C
ATOM	1454	O	GLU	A	197	23.091	-12.242	15.203	1.00	71.96	O

316/396

Figure 3B-27

ATOM	1455	N	ASP	A	198	23.339	-10.008	15.401	1.00	74.81	N
ATOM	1456	CA	ASP	A	198	23.675	-10.015	16.818	1.00	75.86	C
ATOM	1457	CB	ASP	A	198	24.735	-11.079	17.117	1.00	76.32	C
ATOM	1458	CG	ASP	A	198	25.956	-10.936	16.252	1.00	76.85	C
ATOM	1459	OD1	ASP	A	198	26.506	-11.974	15.819	1.00	79.11	O
ATOM	1460	OD2	ASP	A	198	26.367	-9.784	16.012	1.00	75.94	O
ATOM	1461	C	ASP	A	198	24.188	-8.640	17.187	1.00	73.79	C
ATOM	1462	O	ASP	A	198	24.162	-7.718	16.377	1.00	75.37	O
ATOM	1463	N	TYR	A	199	24.655	-8.498	18.412	1.00	71.82	N
ATOM	1464	CA	TYR	A	199	25.157	-7.217	18.855	1.00	70.16	C
ATOM	1465	CB	TYR	A	199	25.379	-7.267	20.361	1.00	70.33	C
ATOM	1466	CG	TYR	A	199	25.657	-5.939	20.998	1.00	70.85	C
ATOM	1467	CD1	TYR	A	199	24.817	-4.855	20.802	1.00	70.07	C
ATOM	1468	CE1	TYR	A	199	25.065	-3.648	21.426	1.00	73.04	C
ATOM	1469	CD2	TYR	A	199	26.745	-5.781	21.827	1.00	73.60	C
ATOM	1470	CE2	TYR	A	199	26.998	-4.590	22.452	1.00	75.48	C
ATOM	1471	CZ	TYR	A	199	26.165	-3.526	22.254	1.00	74.05	C
ATOM	1472	OH	TYR	A	199	26.458	-2.349	22.901	1.00	73.79	O
ATOM	1473	C	TYR	A	199	26.450	-6.876	18.114	1.00	69.40	C
ATOM	1474	O	TYR	A	199	26.672	-5.731	17.736	1.00	70.51	O
ATOM	1475	N	GLY	A	200	27.297	-7.873	17.891	1.00	67.23	N
ATOM	1476	CA	GLY	A	200	28.542	-7.617	17.194	1.00	64.51	C
ATOM	1477	C	GLY	A	200	28.249	-7.009	15.845	1.00	64.24	C
ATOM	1478	O	GLY	A	200	28.823	-5.998	15.461	1.00	62.07	O
ATOM	1479	N	ASP	A	201	27.336	-7.645	15.122	1.00	67.36	N
ATOM	1480	CA	ASP	A	201	26.923	-7.187	13.802	1.00	65.55	C
ATOM	1481	CB	ASP	A	201	25.780	-8.076	13.277	1.00	66.13	C
ATOM	1482	CG	ASP	A	201	25.274	-7.644	11.910	1.00	68.52	C
ATOM	1483	OD1	ASP	A	201	26.106	-7.374	11.015	1.00	67.03	O
ATOM	1484	OD2	ASP	A	201	24.037	-7.586	11.729	1.00	70.04	O
ATOM	1485	C	ASP	A	201	26.475	-5.743	13.958	1.00	62.23	C
ATOM	1486	O	ASP	A	201	26.548	-4.963	13.021	1.00	60.76	O
ATOM	1487	N	TYR	A	202	26.025	-5.399	15.160	1.00	59.66	N
ATOM	1488	CA	TYR	A	202	25.586	-4.045	15.459	1.00	59.85	C
ATOM	1489	CB	TYR	A	202	24.846	-4.026	16.796	1.00	60.50	C
ATOM	1490	CG	TYR	A	202	24.228	-2.694	17.148	1.00	65.60	C
ATOM	1491	CD1	TYR	A	202	23.236	-2.139	16.357	1.00	67.99	C
ATOM	1492	CE1	TYR	A	202	22.651	-0.934	16.681	1.00	69.92	C
ATOM	1493	CD2	TYR	A	202	24.624	-1.999	18.281	1.00	67.65	C
ATOM	1494	CE2	TYR	A	202	24.048	-0.790	18.611	1.00	70.28	C
ATOM	1495	CZ	TYR	A	202	23.060	-0.264	17.807	1.00	71.68	C
ATOM	1496	OH	TYR	A	202	22.477	0.940	18.128	1.00	74.36	O
ATOM	1497	C	TYR	A	202	26.784	-3.068	15.489	1.00	60.40	C
ATOM	1498	O	TYR	A	202	26.861	-2.145	14.676	1.00	60.95	O
ATOM	1499	N	TRP	A	203	27.728	-3.260	16.406	1.00	58.02	N
ATOM	1500	CA	TRP	A	203	28.873	-2.351	16.457	1.00	56.55	C
ATOM	1501	CB	TRP	A	203	29.896	-2.750	17.523	1.00	60.98	C
ATOM	1502	CG	TRP	A	203	29.512	-2.542	18.931	1.00	61.52	C
ATOM	1503	CD2	TRP	A	203	30.069	-3.216	20.056	1.00	63.17	C
ATOM	1504	CE2	TRP	A	203	29.489	-2.655	21.206	1.00	64.57	C
ATOM	1505	CE3	TRP	A	203	31.007	-4.239	20.203	1.00	65.22	C
ATOM	1506	CD1	TRP	A	203	28.638	-1.624	19.422	1.00	61.55	C
ATOM	1507	NE1	TRP	A	203	28.616	-1.684	20.792	1.00	63.07	N
ATOM	1508	CZ2	TRP	A	203	29.818	-3.083	22.493	1.00	65.74	C
ATOM	1509	CZ3	TRP	A	203	31.335	-4.663	21.479	1.00	68.00	C
ATOM	1510	CH2	TRP	A	203	30.742	-4.085	22.608	1.00	66.25	C

317/396

Figure 3B-28

ATOM	1511	C	TRP	A	203	29.623	-2.324	15.141	1.00	54.78	C
ATOM	1512	O	TRP	A	203	30.445	-1.436	14.926	1.00	55.99	O
ATOM	1513	N	ARG	A	204	29.398	-3.324	14.291	1.00	51.29	N
ATOM	1514	CA	ARG	A	204	30.088	-3.365	13.011	1.00	49.16	C
ATOM	1515	CB	ARG	A	204	30.074	-4.766	12.405	1.00	51.67	C
ATOM	1516	CG	ARG	A	204	31.247	-5.675	12.795	1.00	52.09	C
ATOM	1517	CD	ARG	A	204	31.377	-6.853	11.796	1.00	51.97	C
ATOM	1518	NE	ARG	A	204	30.223	-7.757	11.773	1.00	43.95	N
ATOM	1519	CZ	ARG	A	204	29.969	-8.649	12.721	1.00	42.44	C
ATOM	1520	NH1	ARG	A	204	30.789	-8.756	13.753	1.00	39.74	N
ATOM	1521	NH2	ARG	A	204	28.892	-9.419	12.648	1.00	44.63	N
ATOM	1522	C	ARG	A	204	29.314	-2.428	12.130	1.00	48.96	C
ATOM	1523	O	ARG	A	204	29.795	-1.984	11.083	1.00	48.70	O
ATOM	1524	N	GLY	A	205	28.105	-2.122	12.594	1.00	47.24	N
ATOM	1525	CA	GLY	A	205	27.222	-1.232	11.878	1.00	44.49	C
ATOM	1526	C	GLY	A	205	27.900	0.090	11.657	1.00	44.98	C
ATOM	1527	O	GLY	A	205	28.027	0.525	10.523	1.00	47.19	O
ATOM	1528	N	ASP	A	206	28.345	0.708	12.747	1.00	45.54	N
ATOM	1529	CA	ASP	A	206	29.023	2.001	12.733	1.00	46.73	C
ATOM	1530	CB	ASP	A	206	29.982	2.082	13.913	1.00	49.08	C
ATOM	1531	CG	ASP	A	206	30.608	3.455	14.076	1.00	50.37	C
ATOM	1532	OD1	ASP	A	206	31.257	3.974	13.143	1.00	50.22	O
ATOM	1533	OD2	ASP	A	206	30.454	4.016	15.169	1.00	53.85	O
ATOM	1534	C	ASP	A	206	29.787	2.272	11.452	1.00	49.19	C
ATOM	1535	O	ASP	A	206	29.735	3.377	10.910	1.00	50.36	O
ATOM	1536	N	TYR	A	207	30.494	1.261	10.967	1.00	51.18	N
ATOM	1537	CA	TYR	A	207	31.275	1.399	9.746	1.00	55.81	C
ATOM	1538	CB	TYR	A	207	32.385	0.360	9.740	1.00	57.79	C
ATOM	1539	CG	TYR	A	207	33.464	0.632	10.746	1.00	59.74	C
ATOM	1540	CD1	TYR	A	207	33.340	0.188	12.055	1.00	62.44	C
ATOM	1541	CE1	TYR	A	207	34.328	0.439	12.983	1.00	61.21	C
ATOM	1542	CD2	TYR	A	207	34.608	1.339	10.389	1.00	57.39	C
ATOM	1543	CE2	TYR	A	207	35.594	1.594	11.305	1.00	57.25	C
ATOM	1544	CZ	TYR	A	207	35.448	1.142	12.600	1.00	59.36	C
ATOM	1545	OH	TYR	A	207	36.420	1.393	13.524	1.00	59.38	O
ATOM	1546	C	TYR	A	207	30.511	1.300	8.421	1.00	56.71	C
ATOM	1547	O	TYR	A	207	31.069	1.565	7.354	1.00	56.47	O
ATOM	1548	N	GLU	A	208	29.241	0.928	8.485	1.00	57.72	N
ATOM	1549	CA	GLU	A	208	28.432	0.759	7.287	1.00	61.55	C
ATOM	1550	CB	GLU	A	208	27.220	-0.101	7.625	1.00	62.12	C
ATOM	1551	CG	GLU	A	208	26.200	-0.202	6.518	1.00	64.04	C
ATOM	1552	CD	GLU	A	208	25.185	-1.288	6.790	1.00	68.24	C
ATOM	1553	OE1	GLU	A	208	24.828	-1.503	7.973	1.00	70.16	O
ATOM	1554	OE2	GLU	A	208	24.737	-1.925	5.819	1.00	70.18	O
ATOM	1555	C	GLU	A	208	27.968	2.013	6.550	1.00	63.49	C
ATOM	1556	O	GLU	A	208	27.637	3.026	7.165	1.00	65.89	O
ATOM	1557	N	VAL	A	209	27.968	1.926	5.220	1.00	63.73	N
ATOM	1558	CA	VAL	A	209	27.518	3.006	4.346	1.00	65.91	C
ATOM	1559	CB	VAL	A	209	28.689	3.858	3.778	1.00	61.49	C
ATOM	1560	CG1	VAL	A	209	29.599	4.322	4.886	1.00	60.72	C
ATOM	1561	CG2	VAL	A	209	29.440	3.081	2.773	1.00	60.34	C
ATOM	1562	C	VAL	A	209	26.769	2.346	3.176	1.00	70.72	C
ATOM	1563	O	VAL	A	209	27.221	1.336	2.622	1.00	71.60	O
ATOM	1564	N	ASN	A	210	25.615	2.908	2.817	1.00	72.62	N
ATOM	1565	CA	ASN	A	210	24.794	2.370	1.741	1.00	71.13	C
ATOM	1566	CB	ASN	A	210	23.465	1.881	2.300	1.00	70.17	C

318/396

Figure 3B-29

ATOM	1567	CG	ASN	A	210	23.622	0.641	3.141	1.00	72.73	C
ATOM	1568	OD1	ASN	A	210	22.941	0.466	4.159	1.00	73.13	O
ATOM	1569	ND2	ASN	A	210	24.524	-0.242	2.716	1.00	71.94	N
ATOM	1570	C	ASN	A	210	24.536	3.402	0.672	1.00	72.51	C
ATOM	1571	O	ASN	A	210	25.243	3.450	-0.335	1.00	75.02	O
ATOM	1572	N	GLY	A	211	23.517	4.222	0.903	1.00	71.21	N
ATOM	1573	CA	GLY	A	211	23.148	5.258	-0.043	1.00	72.82	C
ATOM	1574	C	GLY	A	211	24.082	5.478	-1.224	1.00	72.35	C
ATOM	1575	O	GLY	A	211	23.686	5.338	-2.377	1.00	72.13	O
ATOM	1576	N	VAL	A	212	25.330	5.825	-0.942	1.00	72.34	N
ATOM	1577	CA	VAL	A	212	26.291	6.073	-1.998	1.00	71.55	C
ATOM	1578	CB	VAL	A	212	27.470	6.885	-1.469	1.00	71.53	C
ATOM	1579	CG1	VAL	A	212	28.370	7.297	-2.628	1.00	70.23	C
ATOM	1580	CG2	VAL	A	212	26.950	8.105	-0.702	1.00	65.70	C
ATOM	1581	C	VAL	A	212	26.804	4.801	-2.661	1.00	72.95	C
ATOM	1582	O	VAL	A	212	26.989	3.768	-2.018	1.00	72.92	O
ATOM	1583	N	ASP	A	213	27.030	4.906	-3.965	1.00	75.31	N
ATOM	1584	CA	ASP	A	213	27.494	3.801	-4.787	1.00	76.76	C
ATOM	1585	CB	ASP	A	213	26.691	3.783	-6.100	1.00	80.98	C
ATOM	1586	CG	ASP	A	213	26.998	2.568	-6.973	1.00	86.17	C
ATOM	1587	OD1	ASP	A	213	26.932	1.428	-6.459	1.00	87.98	O
ATOM	1588	OD2	ASP	A	213	27.293	2.753	-8.180	1.00	87.74	O
ATOM	1589	C	ASP	A	213	28.985	3.959	-5.065	1.00	75.56	C
ATOM	1590	O	ASP	A	213	29.447	5.030	-5.458	1.00	73.59	O
ATOM	1591	N	GLY	A	214	29.737	2.883	-4.862	1.00	74.50	N
ATOM	1592	CA	GLY	A	214	31.169	2.946	-5.087	1.00	73.57	C
ATOM	1593	C	GLY	A	214	31.820	3.377	-3.793	1.00	70.99	C
ATOM	1594	O	GLY	A	214	33.041	3.374	-3.637	1.00	69.46	O
ATOM	1595	N	TYR	A	215	30.962	3.749	-2.855	1.00	68.15	N
ATOM	1596	CA	TYR	A	215	31.391	4.195	-1.551	1.00	64.79	C
ATOM	1597	CB	TYR	A	215	30.995	5.649	-1.351	1.00	59.46	C
ATOM	1598	CG	TYR	A	215	31.848	6.586	-2.160	1.00	59.40	C
ATOM	1599	CD1	TYR	A	215	31.935	6.476	-3.537	1.00	55.99	C
ATOM	1600	CE1	TYR	A	215	32.755	7.312	-4.260	1.00	53.48	C
ATOM	1601	CD2	TYR	A	215	32.602	7.559	-1.541	1.00	60.62	C
ATOM	1602	CE2	TYR	A	215	33.421	8.392	-2.259	1.00	56.89	C
ATOM	1603	CZ	TYR	A	215	33.496	8.265	-3.607	1.00	54.26	C
ATOM	1604	OH	TYR	A	215	34.343	9.098	-4.282	1.00	55.62	O
ATOM	1605	C	TYR	A	215	30.732	3.315	-0.517	1.00	65.16	C
ATOM	1606	O	TYR	A	215	31.009	3.422	0.669	1.00	64.54	O
ATOM	1607	N	ASP	A	216	29.860	2.435	-0.985	1.00	65.56	N
ATOM	1608	CA	ASP	A	216	29.159	1.525	-0.100	1.00	67.79	C
ATOM	1609	CB	ASP	A	216	28.121	0.720	-0.925	1.00	75.68	C
ATOM	1610	CG	ASP	A	216	27.787	-0.660	-0.322	1.00	83.57	C
ATOM	1611	OD1	ASP	A	216	28.403	-1.672	-0.751	1.00	84.69	O
ATOM	1612	OD2	ASP	A	216	26.906	-0.733	0.572	1.00	86.03	O
ATOM	1613	C	ASP	A	216	30.164	0.614	0.610	1.00	64.93	C
ATOM	1614	O	ASP	A	216	31.092	0.101	-0.014	1.00	66.09	O
ATOM	1615	N	TYR	A	217	29.994	0.454	1.923	1.00	61.12	N
ATOM	1616	CA	TYR	A	217	30.841	-0.417	2.746	1.00	57.29	C
ATOM	1617	CB	TYR	A	217	31.753	0.408	3.674	1.00	55.57	C
ATOM	1618	CG	TYR	A	217	32.843	-0.409	4.337	1.00	53.46	C
ATOM	1619	CD1	TYR	A	217	34.077	-0.588	3.730	1.00	49.51	C
ATOM	1620	CE1	TYR	A	217	35.052	-1.412	4.305	1.00	52.26	C
ATOM	1621	CD2	TYR	A	217	32.605	-1.068	5.545	1.00	54.96	C
ATOM	1622	CE2	TYR	A	217	33.563	-1.891	6.126	1.00	52.70	C

319/396

Figure 3B-30

ATOM	1623	CZ	TYR	A	217	34.785	-2.066	5.504	1.00	53.71	C
ATOM	1624	OH	TYR	A	217	35.719	-2.913	6.074	1.00	48.35	O
ATOM	1625	C	TYR	A	217	29.851	-1.257	3.569	1.00	56.27	C
ATOM	1626	O	TYR	A	217	28.896	-0.725	4.133	1.00	56.14	O
ATOM	1627	N	SER	A	218	30.064	-2.565	3.628	1.00	54.25	N
ATOM	1628	CA	SER	A	218	29.147	-3.432	4.354	1.00	53.78	C
ATOM	1629	CB	SER	A	218	28.792	-4.640	3.492	1.00	53.54	C
ATOM	1630	OG	SER	A	218	29.909	-5.067	2.732	1.00	53.19	O
ATOM	1631	C	SER	A	218	29.674	-3.898	5.690	1.00	53.88	C
ATOM	1632	O	SER	A	218	30.866	-3.865	5.934	1.00	55.42	O
ATOM	1633	N	ARG	A	219	28.782	-4.339	6.561	1.00	53.88	N
ATOM	1634	CA	ARG	A	219	29.219	-4.790	7.863	1.00	56.96	C
ATOM	1635	CB	ARG	A	219	28.013	-5.091	8.749	1.00	57.47	C
ATOM	1636	CG	ARG	A	219	27.187	-3.864	9.061	1.00	60.71	C
ATOM	1637	CD	ARG	A	219	26.320	-4.091	10.291	1.00	65.57	C
ATOM	1638	NE	ARG	A	219	25.348	-5.154	10.084	1.00	66.73	N
ATOM	1639	CZ	ARG	A	219	24.279	-5.034	9.308	1.00	67.54	C
ATOM	1640	NH1	ARG	A	219	24.045	-3.893	8.673	1.00	63.53	N
ATOM	1641	NH2	ARG	A	219	23.451	-6.059	9.163	1.00	70.32	N
ATOM	1642	C	ARG	A	219	30.141	-6.001	7.791	1.00	58.68	C
ATOM	1643	O	ARG	A	219	31.226	-5.990	8.353	1.00	59.32	O
ATOM	1644	N	GLY	A	220	29.720	-7.045	7.094	1.00	61.09	N
ATOM	1645	CA	GLY	A	220	30.552	-8.230	7.011	1.00	63.99	C
ATOM	1646	C	GLY	A	220	31.943	-7.912	6.505	1.00	65.02	C
ATOM	1647	O	GLY	A	220	32.891	-8.678	6.719	1.00	64.62	O
ATOM	1648	N	GLN	A	221	32.052	-6.775	5.824	1.00	64.17	N
ATOM	1649	CA	GLN	A	221	33.314	-6.316	5.265	1.00	64.51	C
ATOM	1650	CB	GLN	A	221	33.064	-5.124	4.343	1.00	64.35	C
ATOM	1651	CG	GLN	A	221	34.277	-4.668	3.579	1.00	70.15	C
ATOM	1652	CD	GLN	A	221	34.731	-5.679	2.548	1.00	75.47	C
ATOM	1653	OE1	GLN	A	221	34.019	-5.954	1.582	1.00	78.23	O
ATOM	1654	NE2	GLN	A	221	35.922	-6.242	2.748	1.00	77.57	N
ATOM	1655	C	GLN	A	221	34.285	-5.927	6.387	1.00	65.35	C
ATOM	1656	O	GLN	A	221	35.371	-6.499	6.493	1.00	67.53	O
ATOM	1657	N	LEU	A	222	33.889	-4.965	7.222	1.00	63.93	N
ATOM	1658	CA	LEU	A	222	34.712	-4.503	8.343	1.00	61.04	C
ATOM	1659	CB	LEU	A	222	33.819	-3.884	9.434	1.00	56.82	C
ATOM	1660	CG	LEU	A	222	34.332	-3.175	10.704	1.00	52.84	C
ATOM	1661	CD1	LEU	A	222	34.674	-4.187	11.754	1.00	53.85	C
ATOM	1662	CD2	LEU	A	222	35.517	-2.287	10.398	1.00	49.18	C
ATOM	1663	C	LEU	A	222	35.517	-5.676	8.904	1.00	62.46	C
ATOM	1664	O	LEU	A	222	36.701	-5.533	9.223	1.00	61.59	O
ATOM	1665	N	ILE	A	223	34.892	-6.846	9.007	1.00	60.55	N
ATOM	1666	CA	ILE	A	223	35.634	-7.976	9.519	1.00	60.39	C
ATOM	1667	CB	ILE	A	223	34.796	-9.262	9.621	1.00	59.58	C
ATOM	1668	CG2	ILE	A	223	35.643	-10.382	10.222	1.00	54.78	C
ATOM	1669	CG1	ILE	A	223	33.593	-9.048	10.525	1.00	59.34	C
ATOM	1670	CD1	ILE	A	223	32.874	-10.337	10.845	1.00	60.68	C
ATOM	1671	C	ILE	A	223	36.796	-8.252	8.588	1.00	61.38	C
ATOM	1672	O	ILE	A	223	37.897	-7.766	8.810	1.00	61.82	O
ATOM	1673	N	GLU	A	224	36.533	-9.005	7.528	1.00	64.40	N
ATOM	1674	CA	GLU	A	224	37.568	-9.384	6.576	1.00	67.80	C
ATOM	1675	CB	GLU	A	224	36.959	-10.197	5.431	1.00	74.00	C
ATOM	1676	CG	GLU	A	224	36.070	-9.429	4.480	1.00	81.66	C
ATOM	1677	CD	GLU	A	224	35.749	-10.237	3.233	1.00	86.98	C
ATOM	1678	OE1	GLU	A	224	35.103	-11.304	3.360	1.00	88.38	O

320/396

Figure 3B-31

ATOM	1679	OE2	GLU	A	224	36.154	-9.807	2.128	1.00	90.34	O
ATOM	1680	C	GLU	A	224	38.436	-8.257	6.019	1.00	66.03	C
ATOM	1681	O	GLU	A	224	39.397	-8.505	5.290	1.00	65.29	O
ATOM	1682	N	ASP	A	225	38.113	-7.020	6.365	1.00	64.76	N
ATOM	1683	CA	ASP	A	225	38.926	-5.907	5.907	1.00	63.95	C
ATOM	1684	CB	ASP	A	225	38.068	-4.653	5.735	1.00	69.33	C
ATOM	1685	CG	ASP	A	225	38.376	-3.908	4.447	1.00	71.32	C
ATOM	1686	OD1	ASP	A	225	38.616	-4.582	3.421	1.00	73.49	O
ATOM	1687	OD2	ASP	A	225	38.362	-2.657	4.453	1.00	72.52	O
ATOM	1688	C	ASP	A	225	40.005	-5.700	6.965	1.00	60.44	C
ATOM	1689	O	ASP	A	225	41.069	-5.173	6.673	1.00	58.32	O
ATOM	1690	N	VAL	A	226	39.706	-6.123	8.194	1.00	58.34	N
ATOM	1691	CA	VAL	A	226	40.644	-6.053	9.315	1.00	56.93	C
ATOM	1692	CB	VAL	A	226	39.933	-6.168	10.664	1.00	57.55	C
ATOM	1693	CG1	VAL	A	226	40.955	-6.234	11.781	1.00	56.37	C
ATOM	1694	CG2	VAL	A	226	39.023	-4.988	10.866	1.00	60.52	C
ATOM	1695	C	VAL	A	226	41.564	-7.255	9.186	1.00	56.72	C
ATOM	1696	O	VAL	A	226	42.772	-7.159	9.384	1.00	54.50	O
ATOM	1697	N	GLU	A	227	40.956	-8.395	8.870	1.00	58.07	N
ATOM	1698	CA	GLU	A	227	41.666	-9.646	8.656	1.00	59.71	C
ATOM	1699	CB	GLU	A	227	40.737	-10.658	7.984	1.00	60.33	C
ATOM	1700	CG	GLU	A	227	39.364	-10.789	8.619	1.00	64.40	C
ATOM	1701	CD	GLU	A	227	39.342	-11.771	9.760	1.00	69.25	C
ATOM	1702	OE1	GLU	A	227	38.241	-12.090	10.267	1.00	70.06	O
ATOM	1703	OE2	GLU	A	227	40.436	-12.226	10.150	1.00	74.88	O
ATOM	1704	C	GLU	A	227	42.831	-9.356	7.709	1.00	61.17	C
ATOM	1705	O	GLU	A	227	43.997	-9.460	8.086	1.00	62.26	O
ATOM	1706	N	HIS	A	228	42.491	-8.987	6.477	1.00	61.01	N
ATOM	1707	CA	HIS	A	228	43.468	-8.679	5.436	1.00	61.28	C
ATOM	1708	CB	HIS	A	228	42.734	-8.117	4.217	1.00	66.35	C
ATOM	1709	CG	HIS	A	228	43.632	-7.738	3.077	1.00	73.37	C
ATOM	1710	CD2	HIS	A	228	43.713	-8.214	1.812	1.00	75.61	C
ATOM	1711	ND1	HIS	A	228	44.557	-6.718	3.160	1.00	77.96	N
ATOM	1712	CE1	HIS	A	228	45.167	-6.579	1.996	1.00	76.78	C
ATOM	1713	NE2	HIS	A	228	44.673	-7.474	1.161	1.00	78.18	N
ATOM	1714	C	HIS	A	228	44.544	-7.702	5.900	1.00	59.56	C
ATOM	1715	O	HIS	A	228	45.735	-7.975	5.822	1.00	62.16	O
ATOM	1716	N	THR	A	229	44.122	-6.552	6.387	1.00	59.04	N
ATOM	1717	CA	THR	A	229	45.056	-5.540	6.857	1.00	57.06	C
ATOM	1718	CB	THR	A	229	44.262	-4.262	7.273	1.00	56.62	C
ATOM	1719	OG1	THR	A	229	45.165	-3.208	7.612	1.00	61.73	O
ATOM	1720	CG2	THR	A	229	43.375	-4.549	8.454	1.00	52.20	C
ATOM	1721	C	THR	A	229	45.928	-6.053	8.025	1.00	54.80	C
ATOM	1722	O	THR	A	229	46.984	-5.499	8.312	1.00	49.71	O
ATOM	1723	N	PHE	A	230	45.486	-7.123	8.682	1.00	55.41	N
ATOM	1724	CA	PHE	A	230	46.219	-7.688	9.814	1.00	56.87	C
ATOM	1725	CB	PHE	A	230	45.302	-8.574	10.655	1.00	54.77	C
ATOM	1726	CG	PHE	A	230	45.930	-9.045	11.942	1.00	56.26	C
ATOM	1727	CD1	PHE	A	230	46.582	-8.152	12.783	1.00	57.11	C
ATOM	1728	CD2	PHE	A	230	45.822	-10.363	12.342	1.00	53.63	C
ATOM	1729	CE1	PHE	A	230	47.106	-8.567	13.992	1.00	54.48	C
ATOM	1730	CE2	PHE	A	230	46.345	-10.775	13.553	1.00	52.47	C
ATOM	1731	CZ	PHE	A	230	46.985	-9.877	14.375	1.00	52.45	C
ATOM	1732	C	PHE	A	230	47.436	-8.497	9.397	1.00	58.80	C
ATOM	1733	O	PHE	A	230	48.459	-8.495	10.090	1.00	56.25	O
ATOM	1734	N	GLU	A	231	47.307	-9.199	8.272	1.00	62.23	N

321/396

Figure 3B-32

ATOM	1735	CA	GLU	A	231	48.383	-10.021	7.725	1.00	63.27	C
ATOM	1736	CB	GLU	A	231	47.988	-10.580	6.359	1.00	66.92	C
ATOM	1737	CG	GLU	A	231	46.733	-11.419	6.381	1.00	74.13	C
ATOM	1738	CD	GLU	A	231	46.913	-12.679	7.185	1.00	78.94	C
ATOM	1739	OE1	GLU	A	231	47.611	-13.598	6.708	1.00	81.69	O
ATOM	1740	OE2	GLU	A	231	46.364	-12.748	8.302	1.00	84.12	O
ATOM	1741	C	GLU	A	231	49.646	-9.192	7.568	1.00	62.69	C
ATOM	1742	O	GLU	A	231	50.689	-9.538	8.103	1.00	66.41	O
ATOM	1743	N	GLU	A	232	49.563	-8.091	6.840	1.00	59.28	N
ATOM	1744	CA	GLU	A	232	50.742	-7.274	6.649	1.00	58.63	C
ATOM	1745	CB	GLU	A	232	50.447	-6.156	5.651	1.00	61.86	C
ATOM	1746	CG	GLU	A	232	50.314	-6.632	4.206	1.00	67.06	C
ATOM	1747	CD	GLU	A	232	49.901	-5.522	3.246	1.00	66.43	C
ATOM	1748	OE1	GLU	A	232	48.733	-5.071	3.316	1.00	65.77	O
ATOM	1749	OE2	GLU	A	232	50.750	-5.106	2.426	1.00	62.67	O
ATOM	1750	C	GLU	A	232	51.253	-6.682	7.953	1.00	58.36	C
ATOM	1751	O	GLU	A	232	52.334	-6.098	7.990	1.00	61.89	O
ATOM	1752	N	ILE	A	233	50.490	-6.830	9.028	1.00	55.56	N
ATOM	1753	CA	ILE	A	233	50.904	-6.269	10.308	1.00	56.53	C
ATOM	1754	CB	ILE	A	233	49.679	-5.798	11.144	1.00	57.82	C
ATOM	1755	CG2	ILE	A	233	50.053	-5.675	12.631	1.00	54.26	C
ATOM	1756	CG1	ILE	A	233	49.190	-4.444	10.636	1.00	54.98	C
ATOM	1757	CD1	ILE	A	233	50.154	-3.317	10.930	1.00	53.56	C
ATOM	1758	C	ILE	A	233	51.706	-7.250	11.139	1.00	57.76	C
ATOM	1759	O	ILE	A	233	52.533	-6.844	11.957	1.00	56.47	O
ATOM	1760	N	LYS	A	234	51.462	-8.538	10.919	1.00	57.21	N
ATOM	1761	CA	LYS	A	234	52.139	-9.585	11.666	1.00	57.09	C
ATOM	1762	CB	LYS	A	234	51.638	-10.950	11.226	1.00	52.71	C
ATOM	1763	CG	LYS	A	234	50.224	-11.206	11.667	1.00	53.95	C
ATOM	1764	CD	LYS	A	234	49.800	-12.612	11.359	1.00	54.31	C
ATOM	1765	CE	LYS	A	234	48.526	-12.938	12.089	1.00	59.07	C
ATOM	1766	NZ	LYS	A	234	48.197	-14.386	12.018	1.00	65.50	N
ATOM	1767	C	LYS	A	234	53.657	-9.543	11.627	1.00	60.34	C
ATOM	1768	O	LYS	A	234	54.287	-9.424	12.671	1.00	64.94	O
ATOM	1769	N	PRO	A	235	54.275	-9.651	10.440	1.00	60.44	N
ATOM	1770	CD	PRO	A	235	53.749	-9.821	9.074	1.00	61.42	C
ATOM	1771	CA	PRO	A	235	55.739	-9.601	10.431	1.00	60.60	C
ATOM	1772	CB	PRO	A	235	56.052	-9.242	8.985	1.00	58.52	C
ATOM	1773	CG	PRO	A	235	55.021	-10.047	8.252	1.00	60.47	C
ATOM	1774	C	PRO	A	235	56.296	-8.583	11.430	1.00	61.45	C
ATOM	1775	O	PRO	A	235	56.966	-8.949	12.393	1.00	63.86	O
ATOM	1776	N	LEU	A	236	55.995	-7.310	11.216	1.00	60.05	N
ATOM	1777	CA	LEU	A	236	56.470	-6.261	12.105	1.00	57.11	C
ATOM	1778	CB	LEU	A	236	55.863	-4.927	11.699	1.00	56.28	C
ATOM	1779	CG	LEU	A	236	56.172	-3.786	12.656	1.00	52.87	C
ATOM	1780	CD1	LEU	A	236	57.654	-3.653	12.784	1.00	50.99	C
ATOM	1781	CD2	LEU	A	236	55.564	-2.510	12.142	1.00	53.88	C
ATOM	1782	C	LEU	A	236	56.170	-6.510	13.579	1.00	56.87	C
ATOM	1783	O	LEU	A	236	56.872	-5.995	14.450	1.00	59.80	O
ATOM	1784	N	TYR	A	237	55.123	-7.277	13.865	1.00	54.26	N
ATOM	1785	CA	TYR	A	237	54.761	-7.567	15.253	1.00	53.98	C
ATOM	1786	CB	TYR	A	237	53.333	-8.110	15.362	1.00	45.72	C
ATOM	1787	CG	TYR	A	237	52.927	-8.485	16.780	1.00	39.57	C
ATOM	1788	CD1	TYR	A	237	53.207	-7.641	17.848	1.00	35.36	C
ATOM	1789	CE1	TYR	A	237	52.818	-7.961	19.140	1.00	31.97	C
ATOM	1790	CD2	TYR	A	237	52.237	-9.673	17.046	1.00	38.02	C

322/396

Figure 3B-33

ATOM	1791	CE2	TYR	A	237	51.838	-10.007	18.342	1.00	30.04	C
ATOM	1792	CZ	TYR	A	237	52.137	-9.144	19.387	1.00	32.86	C
ATOM	1793	OH	TYR	A	237	51.789	-9.467	20.686	1.00	30.71	O
ATOM	1794	C	TYR	A	237	55.709	-8.604	15.795	1.00	58.09	C
ATOM	1795	O	TYR	A	237	56.393	-8.378	16.792	1.00	59.03	O
ATOM	1796	N	GLU	A	238	55.741	-9.749	15.121	1.00	61.89	N
ATOM	1797	CA	GLU	A	238	56.599	-10.841	15.522	1.00	61.47	C
ATOM	1798	CB	GLU	A	238	56.682	-11.899	14.419	1.00	62.17	C
ATOM	1799	CG	GLU	A	238	55.319	-12.525	14.081	1.00	64.31	C
ATOM	1800	CD	GLU	A	238	55.426	-13.755	13.185	1.00	66.39	C
ATOM	1801	OE1	GLU	A	238	55.356	-14.881	13.721	1.00	63.21	O
ATOM	1802	OE2	GLU	A	238	55.588	-13.596	11.951	1.00	66.18	O
ATOM	1803	C	GLU	A	238	57.975	-10.326	15.887	1.00	60.33	C
ATOM	1804	O	GLU	A	238	58.368	-10.427	17.041	1.00	64.21	O
ATOM	1805	N	HIS	A	239	58.709	-9.743	14.950	1.00	56.57	N
ATOM	1806	CA	HIS	A	239	60.033	-9.272	15.329	1.00	57.70	C
ATOM	1807	CB	HIS	A	239	60.780	-8.635	14.154	1.00	59.10	C
ATOM	1808	CG	HIS	A	239	61.094	-9.590	13.045	1.00	60.15	C
ATOM	1809	CD2	HIS	A	239	60.432	-10.679	12.592	1.00	59.67	C
ATOM	1810	ND1	HIS	A	239	62.172	-9.421	12.201	1.00	61.87	N
ATOM	1811	CE1	HIS	A	239	62.155	-10.362	11.276	1.00	63.22	C
ATOM	1812	NE2	HIS	A	239	61.108	-11.140	11.489	1.00	60.40	N
ATOM	1813	C	HIS	A	239	59.983	-8.290	16.486	1.00	57.87	C
ATOM	1814	O	HIS	A	239	60.963	-8.130	17.206	1.00	61.27	O
ATOM	1815	N	LEU	A	240	58.848	-7.634	16.683	1.00	56.28	N
ATOM	1816	CA	LEU	A	240	58.740	-6.683	17.781	1.00	54.51	C
ATOM	1817	CB	LEU	A	240	57.635	-5.655	17.489	1.00	54.60	C
ATOM	1818	CG	LEU	A	240	57.331	-4.476	18.446	1.00	55.42	C
ATOM	1819	CD1	LEU	A	240	56.329	-4.921	19.531	1.00	52.34	C
ATOM	1820	CD2	LEU	A	240	58.633	-3.895	19.035	1.00	46.06	C
ATOM	1821	C	LEU	A	240	58.449	-7.441	19.063	1.00	53.54	C
ATOM	1822	O	LEU	A	240	58.878	-7.037	20.136	1.00	52.42	O
ATOM	1823	N	HIS	A	241	57.731	-8.553	18.935	1.00	55.19	N
ATOM	1824	CA	HIS	A	241	57.361	-9.404	20.067	1.00	57.01	C
ATOM	1825	CB	HIS	A	241	56.127	-10.231	19.700	1.00	59.75	C
ATOM	1826	CG	HIS	A	241	55.924	-11.440	20.561	1.00	63.95	C
ATOM	1827	CD2	HIS	A	241	55.019	-11.698	21.536	1.00	63.16	C
ATOM	1828	ND1	HIS	A	241	56.695	-12.576	20.441	1.00	65.55	N
ATOM	1829	CE1	HIS	A	241	56.271	-13.484	21.306	1.00	64.39	C
ATOM	1830	NE2	HIS	A	241	55.256	-12.976	21.981	1.00	63.71	N
ATOM	1831	C	HIS	A	241	58.499	-10.331	20.480	1.00	56.84	C
ATOM	1832	O	HIS	A	241	58.769	-10.506	21.661	1.00	54.30	O
ATOM	1833	N	ALA	A	242	59.152	-10.925	19.492	1.00	58.32	N
ATOM	1834	CA	ALA	A	242	60.267	-11.819	19.729	1.00	61.10	C
ATOM	1835	CB	ALA	A	242	60.560	-12.623	18.474	1.00	62.29	C
ATOM	1836	C	ALA	A	242	61.508	-11.030	20.154	1.00	62.00	C
ATOM	1837	O	ALA	A	242	62.506	-11.614	20.588	1.00	64.21	O
ATOM	1838	N	TYR	A	243	61.457	-9.709	20.015	1.00	60.46	N
ATOM	1839	CA	TYR	A	243	62.578	-8.874	20.423	1.00	61.76	C
ATOM	1840	CB	TYR	A	243	62.632	-7.576	19.637	1.00	59.98	C
ATOM	1841	CG	TYR	A	243	63.454	-6.474	20.305	1.00	59.25	C
ATOM	1842	CD1	TYR	A	243	64.756	-6.203	19.901	1.00	58.34	C
ATOM	1843	CE1	TYR	A	243	65.476	-5.144	20.445	1.00	59.34	C
ATOM	1844	CD2	TYR	A	243	62.896	-5.658	21.292	1.00	60.17	C
ATOM	1845	CE2	TYR	A	243	63.609	-4.598	21.847	1.00	60.92	C
ATOM	1846	CZ	TYR	A	243	64.896	-4.339	21.412	1.00	61.57	C

323/396

Figure 3B-34

ATOM	1847	OH	TYR	A	243	65.574	-3.235	21.889	1.00	58.65	O
ATOM	1848	C	TYR	A	243	62.432	-8.507	21.879	1.00	65.72	C
ATOM	1849	O	TYR	A	243	63.425	-8.275	22.561	1.00	69.38	O
ATOM	1850	N	VAL	A	244	61.195	-8.420	22.356	1.00	67.07	N
ATOM	1851	CA	VAL	A	244	60.980	-8.051	23.746	1.00	68.32	C
ATOM	1852	CB	VAL	A	244	59.762	-7.117	23.927	1.00	68.92	C
ATOM	1853	CG1	VAL	A	244	59.805	-5.995	22.891	1.00	64.93	C
ATOM	1854	CG2	VAL	A	244	58.476	-7.921	23.870	1.00	65.37	C
ATOM	1855	C	VAL	A	244	60.780	-9.272	24.614	1.00	69.10	C
ATOM	1856	O	VAL	A	244	60.559	-9.151	25.817	1.00	71.21	O
ATOM	1857	N	ARG	A	245	60.817	-10.452	24.003	1.00	67.91	N
ATOM	1858	CA	ARG	A	245	60.699	-11.679	24.781	1.00	65.48	C
ATOM	1859	CB	ARG	A	245	60.308	-12.863	23.906	1.00	61.77	C
ATOM	1860	CG	ARG	A	245	61.315	-13.244	22.830	1.00	61.82	C
ATOM	1861	CD	ARG	A	245	60.725	-14.421	22.132	1.00	58.08	C
ATOM	1862	NE	ARG	A	245	59.885	-15.081	23.121	1.00	56.33	N
ATOM	1863	CZ	ARG	A	245	58.977	-16.002	22.842	1.00	59.31	C
ATOM	1864	NH1	ARG	A	245	58.267	-16.538	23.828	1.00	57.50	N
ATOM	1865	NH2	ARG	A	245	58.778	-16.379	21.582	1.00	60.25	N
ATOM	1866	C	ARG	A	245	62.132	-11.812	25.234	1.00	64.87	C
ATOM	1867	O	ARG	A	245	62.444	-12.435	26.242	1.00	65.27	O
ATOM	1868	N	ALA	A	246	62.997	-11.184	24.454	1.00	62.96	N
ATOM	1869	CA	ALA	A	246	64.405	-11.158	24.738	1.00	61.38	C
ATOM	1870	CB	ALA	A	246	65.158	-10.619	23.544	1.00	61.77	C
ATOM	1871	C	ALA	A	246	64.582	-10.241	25.941	1.00	60.94	C
ATOM	1872	O	ALA	A	246	64.510	-10.697	27.073	1.00	61.37	O
ATOM	1873	N	LYS	A	247	64.774	-8.949	25.692	1.00	59.89	N
ATOM	1874	CA	LYS	A	247	64.991	-7.972	26.752	1.00	59.24	C
ATOM	1875	CB	LYS	A	247	64.910	-6.558	26.181	1.00	57.62	C
ATOM	1876	CG	LYS	A	247	65.866	-6.373	25.012	1.00	57.81	C
ATOM	1877	CD	LYS	A	247	66.315	-4.946	24.837	1.00	58.18	C
ATOM	1878	CE	LYS	A	247	67.057	-4.452	26.062	1.00	62.18	C
ATOM	1879	NZ	LYS	A	247	67.871	-3.228	25.782	1.00	63.56	N
ATOM	1880	C	LYS	A	247	64.083	-8.109	27.964	1.00	61.49	C
ATOM	1881	O	LYS	A	247	64.257	-7.392	28.956	1.00	60.71	O
ATOM	1882	N	LEU	A	248	63.115	-9.024	27.884	1.00	63.77	N
ATOM	1883	CA	LEU	A	248	62.209	-9.286	29.004	1.00	65.27	C
ATOM	1884	CB	LEU	A	248	60.800	-9.660	28.532	1.00	58.89	C
ATOM	1885	CG	LEU	A	248	59.678	-8.688	28.921	1.00	53.15	C
ATOM	1886	CD1	LEU	A	248	58.492	-9.475	29.423	1.00	53.27	C
ATOM	1887	CD2	LEU	A	248	60.139	-7.748	30.008	1.00	51.34	C
ATOM	1888	C	LEU	A	248	62.811	-10.438	29.800	1.00	69.92	C
ATOM	1889	O	LEU	A	248	62.672	-10.491	31.026	1.00	74.06	O
ATOM	1890	N	MET	A	249	63.469	-11.367	29.104	1.00	71.38	N
ATOM	1891	CA	MET	A	249	64.139	-12.475	29.778	1.00	71.40	C
ATOM	1892	CB	MET	A	249	64.768	-13.450	28.771	1.00	71.08	C
ATOM	1893	CG	MET	A	249	63.764	-14.306	28.000	1.00	75.05	C
ATOM	1894	SD	MET	A	249	64.491	-15.522	26.839	1.00	75.40	S
ATOM	1895	CE	MET	A	249	65.645	-14.475	25.891	1.00	70.04	C
ATOM	1896	C	MET	A	249	65.244	-11.810	30.598	1.00	70.89	C
ATOM	1897	O	MET	A	249	65.429	-12.118	31.772	1.00	70.85	O
ATOM	1898	N	ASN	A	250	65.946	-10.871	29.965	1.00	69.30	N
ATOM	1899	CA	ASN	A	250	67.044	-10.134	30.581	1.00	69.02	C
ATOM	1900	CB	ASN	A	250	67.536	-9.036	29.640	1.00	71.67	C
ATOM	1901	CG	ASN	A	250	68.866	-8.439	30.079	1.00	74.32	C
ATOM	1902	OD1	ASN	A	250	69.931	-8.965	29.751	1.00	77.36	O

324/396

Figure 3B-35

ATOM	1903	ND2	ASN	A	250	68.810	-7.343	30.831	1.00	75.43	N
ATOM	1904	C	ASN	A	250	66.689	-9.487	31.905	1.00	70.36	C
ATOM	1905	O	ASN	A	250	67.555	-8.896	32.548	1.00	71.97	O
ATOM	1906	N	ALA	A	251	65.427	-9.575	32.313	1.00	70.61	N
ATOM	1907	CA	ALA	A	251	65.007	-8.969	33.571	1.00	70.24	C
ATOM	1908	CB	ALA	A	251	64.475	-7.563	33.322	1.00	71.23	C
ATOM	1909	C	ALA	A	251	63.962	-9.808	34.280	1.00	69.98	C
ATOM	1910	O	ALA	A	251	63.265	-9.323	35.167	1.00	71.38	O
ATOM	1911	N	TYR	A	252	63.856	-11.066	33.868	1.00	70.50	N
ATOM	1912	CA	TYR	A	252	62.931	-12.047	34.449	1.00	72.91	C
ATOM	1913	CB	TYR	A	252	61.497	-11.808	33.961	1.00	73.75	C
ATOM	1914	CG	TYR	A	252	60.895	-10.481	34.366	1.00	73.49	C
ATOM	1915	CD1	TYR	A	252	60.486	-10.245	35.666	1.00	71.78	C
ATOM	1916	CE1	TYR	A	252	59.943	-9.024	36.036	1.00	74.36	C
ATOM	1917	CD2	TYR	A	252	60.748	-9.458	33.441	1.00	76.70	C
ATOM	1918	CE2	TYR	A	252	60.208	-8.233	33.801	1.00	77.61	C
ATOM	1919	CZ	TYR	A	252	59.807	-8.019	35.099	1.00	75.65	C
ATOM	1920	OH	TYR	A	252	59.276	-6.798	35.449	1.00	73.36	O
ATOM	1921	C	TYR	A	252	63.401	-13.433	33.976	1.00	73.71	C
ATOM	1922	O	TYR	A	252	62.595	-14.257	33.523	1.00	73.18	O
ATOM	1923	N	PRO	A	253	64.718	-13.709	34.106	1.00	72.58	N
ATOM	1924	CD	PRO	A	253	65.613	-12.969	35.022	1.00	69.34	C
ATOM	1925	CA	PRO	A	253	65.345	-14.969	33.696	1.00	68.49	C
ATOM	1926	CB	PRO	A	253	66.796	-14.739	34.049	1.00	67.07	C
ATOM	1927	CG	PRO	A	253	66.668	-13.989	35.347	1.00	65.60	C
ATOM	1928	C	PRO	A	253	64.763	-16.159	34.426	1.00	68.51	C
ATOM	1929	O	PRO	A	253	64.513	-16.090	35.619	1.00	63.86	O
ATOM	1930	N	SER	A	254	64.560	-17.249	33.697	1.00	73.39	N
ATOM	1931	CA	SER	A	254	64.003	-18.483	34.256	1.00	79.09	C
ATOM	1932	CB	SER	A	254	64.458	-18.691	35.697	1.00	77.27	C
ATOM	1933	OG	SER	A	254	63.592	-18.004	36.582	1.00	71.50	O
ATOM	1934	C	SER	A	254	62.484	-18.422	34.254	1.00	83.34	C
ATOM	1935	O	SER	A	254	61.802	-19.372	34.665	1.00	83.32	O
ATOM	1936	N	TYR	A	255	61.963	-17.291	33.790	1.00	86.45	N
ATOM	1937	CA	TYR	A	255	60.528	-17.069	33.757	1.00	86.90	C
ATOM	1938	CB	TYR	A	255	60.217	-15.752	34.478	1.00	85.34	C
ATOM	1939	CG	TYR	A	255	60.099	-15.897	35.982	1.00	82.73	C
ATOM	1940	CD1	TYR	A	255	60.711	-14.995	36.842	1.00	81.92	C
ATOM	1941	CE1	TYR	A	255	60.558	-15.102	38.217	1.00	82.24	C
ATOM	1942	CD2	TYR	A	255	59.333	-16.914	36.537	1.00	83.03	C
ATOM	1943	CE2	TYR	A	255	59.171	-17.028	37.905	1.00	82.79	C
ATOM	1944	CZ	TYR	A	255	59.782	-16.121	38.743	1.00	83.22	C
ATOM	1945	OH	TYR	A	255	59.596	-16.232	40.107	1.00	82.50	O
ATOM	1946	C	TYR	A	255	59.916	-17.080	32.355	1.00	87.71	C
ATOM	1947	O	TYR	A	255	58.749	-17.440	32.185	1.00	89.12	O
ATOM	1948	N	ILE	A	256	60.694	-16.716	31.343	1.00	87.10	N
ATOM	1949	CA	ILE	A	256	60.142	-16.701	29.998	1.00	87.03	C
ATOM	1950	CB	ILE	A	256	59.951	-15.253	29.523	1.00	88.79	C
ATOM	1951	CG2	ILE	A	256	58.980	-15.216	28.353	1.00	87.62	C
ATOM	1952	CG1	ILE	A	256	59.392	-14.408	30.669	1.00	87.68	C
ATOM	1953	CD1	ILE	A	256	59.363	-12.944	30.370	1.00	89.66	C
ATOM	1954	C	ILE	A	256	60.976	-17.471	28.974	1.00	86.05	C
ATOM	1955	O	ILE	A	256	62.175	-17.219	28.799	1.00	85.44	O
ATOM	1956	N	SER	A	257	60.319	-18.412	28.300	1.00	83.27	N
ATOM	1957	CA	SER	A	257	60.954	-19.248	27.283	1.00	83.81	C
ATOM	1958	CB	SER	A	257	60.017	-20.392	26.892	1.00	82.50	C

325/396

Figure 3B-36

ATOM	1959	OG	SER A 257	60.379	-20.928	25.630	1.00	81.36	O
ATOM	1960	C	SER A 257	61.338	-18.495	26.015	1.00	83.63	C
ATOM	1961	O	SER A 257	60.541	-17.736	25.474	1.00	86.21	O
ATOM	1962	N	PRO A 258	62.562	-18.702	25.511	1.00	82.26	N
ATOM	1963	CD	PRO A 258	63.748	-19.356	26.087	1.00	81.07	C
ATOM	1964	CA	PRO A 258	62.908	-17.975	24.287	1.00	80.65	C
ATOM	1965	CB	PRO A 258	64.407	-18.244	24.132	1.00	80.26	C
ATOM	1966	CG	PRO A 258	64.864	-18.514	25.530	1.00	79.48	C
ATOM	1967	C	PRO A 258	62.106	-18.505	23.092	1.00	79.67	C
ATOM	1968	O	PRO A 258	62.569	-18.424	21.951	1.00	78.57	O
ATOM	1969	N	ILE A 259	60.909	-19.041	23.349	1.00	78.01	N
ATOM	1970	CA	ILE A 259	60.086	-19.583	22.266	1.00	77.75	C
ATOM	1971	CB	ILE A 259	60.593	-21.001	21.883	1.00	76.74	C
ATOM	1972	CG2	ILE A 259	59.991	-22.042	22.819	1.00	74.77	C
ATOM	1973	CG1	ILE A 259	60.212	-21.327	20.440	1.00	75.99	C
ATOM	1974	CD1	ILE A 259	60.508	-22.740	20.036	1.00	74.13	C
ATOM	1975	C	ILE A 259	58.552	-19.654	22.507	1.00	77.52	C
ATOM	1976	O	ILE A 259	57.836	-20.313	21.748	1.00	76.46	O
ATOM	1977	N	GLY A 260	58.033	-18.975	23.528	1.00	76.67	N
ATOM	1978	CA	GLY A 260	56.598	-19.061	23.763	1.00	76.02	C
ATOM	1979	C	GLY A 260	55.872	-17.929	24.472	1.00	75.64	C
ATOM	1980	O	GLY A 260	55.828	-17.881	25.697	1.00	77.66	O
ATOM	1981	N	CYS A 261	55.296	-17.029	23.678	1.00	75.27	N
ATOM	1982	CA	CYS A 261	54.515	-15.871	24.131	1.00	72.48	C
ATOM	1983	CB	CYS A 261	53.067	-16.088	23.745	1.00	74.82	C
ATOM	1984	SG	CYS A 261	52.503	-17.728	24.132	1.00	83.26	S
ATOM	1985	C	CYS A 261	54.571	-15.492	25.597	1.00	69.76	C
ATOM	1986	O	CYS A 261	54.031	-16.190	26.445	1.00	69.00	O
ATOM	1987	N	LEU A 262	55.184	-14.346	25.873	1.00	68.77	N
ATOM	1988	CA	LEU A 262	55.354	-13.831	27.232	1.00	68.21	C
ATOM	1989	CB	LEU A 262	55.746	-12.349	27.190	1.00	66.72	C
ATOM	1990	CG	LEU A 262	56.693	-11.855	26.096	1.00	66.85	C
ATOM	1991	CD1	LEU A 262	55.905	-11.517	24.835	1.00	66.26	C
ATOM	1992	CD2	LEU A 262	57.413	-10.623	26.584	1.00	65.61	C
ATOM	1993	C	LEU A 262	54.161	-13.973	28.178	1.00	68.60	C
ATOM	1994	O	LEU A 262	53.022	-14.179	27.758	1.00	68.47	O
ATOM	1995	N	PRO A 263	54.429	-13.889	29.490	1.00	70.05	N
ATOM	1996	CD	PRO A 263	55.771	-14.086	30.079	1.00	69.53	C
ATOM	1997	CA	PRO A 263	53.380	-13.993	30.513	1.00	68.95	C
ATOM	1998	CB	PRO A 263	54.172	-14.344	31.782	1.00	70.73	C
ATOM	1999	CG	PRO A 263	55.547	-13.754	31.520	1.00	68.60	C
ATOM	2000	C	PRO A 263	52.586	-12.675	30.619	1.00	65.07	C
ATOM	2001	O	PRO A 263	53.163	-11.585	30.642	1.00	63.79	O
ATOM	2002	N	ALA A 264	51.266	-12.790	30.692	1.00	60.47	N
ATOM	2003	CA	ALA A 264	50.370	-11.632	30.739	1.00	58.97	C
ATOM	2004	CB	ALA A 264	48.931	-12.122	30.922	1.00	55.80	C
ATOM	2005	C	ALA A 264	50.628	-10.484	31.720	1.00	59.26	C
ATOM	2006	O	ALA A 264	50.110	-9.386	31.524	1.00	59.29	O
ATOM	2007	N	HIS A 265	51.425	-10.699	32.757	1.00	58.72	N
ATOM	2008	CA	HIS A 265	51.620	-9.642	33.743	1.00	58.48	C
ATOM	2009	CB	HIS A 265	51.508	-10.241	35.144	1.00	61.83	C
ATOM	2010	CG	HIS A 265	52.503	-11.327	35.414	1.00	65.11	C
ATOM	2011	CD2	HIS A 265	53.433	-11.463	36.389	1.00	64.41	C
ATOM	2012	ND1	HIS A 265	52.636	-12.435	34.604	1.00	64.27	N
ATOM	2013	CE1	HIS A 265	53.606	-13.201	35.066	1.00	64.10	C
ATOM	2014	NE2	HIS A 265	54.106	-12.633	36.149	1.00	62.22	N

326/396

Figure 3B-37

ATOM	2015	C	HIS	A	265	52.877	-8.792	33.674	1.00	58.09	C
ATOM	2016	O	HIS	A	265	53.084	-7.935	34.536	1.00	56.62	O
ATOM	2017	N	LEU	A	266	53.719	-9.009	32.670	1.00	59.31	N
ATOM	2018	CA	LEU	A	266	54.956	-8.228	32.565	1.00	61.28	C
ATOM	2019	CB	LEU	A	266	56.174	-9.156	32.409	1.00	60.90	C
ATOM	2020	CG	LEU	A	266	56.218	-10.528	33.101	1.00	59.94	C
ATOM	2021	CD1	LEU	A	266	57.538	-11.183	32.769	1.00	59.04	C
ATOM	2022	CD2	LEU	A	266	56.056	-10.401	34.609	1.00	59.66	C
ATOM	2023	C	LEU	A	266	54.876	-7.302	31.359	1.00	61.80	C
ATOM	2024	O	LEU	A	266	55.863	-6.668	30.973	1.00	61.47	O
ATOM	2025	N	LEU	A	267	53.678	-7.214	30.794	1.00	60.58	N
ATOM	2026	CA	LEU	A	267	53.437	-6.419	29.609	1.00	58.61	C
ATOM	2027	CB	LEU	A	267	52.141	-6.880	28.974	1.00	54.91	C
ATOM	2028	CG	LEU	A	267	52.351	-8.304	28.481	1.00	52.58	C
ATOM	2029	CD1	LEU	A	267	51.044	-8.969	28.068	1.00	51.95	C
ATOM	2030	CD2	LEU	A	267	53.330	-8.235	27.347	1.00	50.68	C
ATOM	2031	C	LEU	A	267	53.448	-4.907	29.712	1.00	60.26	C
ATOM	2032	O	LEU	A	267	53.434	-4.237	28.686	1.00	64.11	O
ATOM	2033	N	GLY	A	268	53.482	-4.352	30.919	1.00	59.26	N
ATOM	2034	CA	GLY	A	268	53.516	-2.901	31.034	1.00	56.89	C
ATOM	2035	C	GLY	A	268	52.246	-2.251	31.549	1.00	56.41	C
ATOM	2036	O	GLY	A	268	52.218	-1.041	31.768	1.00	53.29	O
ATOM	2037	N	ASP	A	269	51.193	-3.051	31.709	1.00	57.22	N
ATOM	2038	CA	ASP	A	269	49.912	-2.584	32.241	1.00	58.39	C
ATOM	2039	CB	ASP	A	269	49.356	-1.387	31.442	1.00	64.11	C
ATOM	2040	CG	ASP	A	269	49.064	-1.716	29.992	1.00	67.57	C
ATOM	2041	OD1	ASP	A	269	48.566	-0.814	29.278	1.00	66.45	O
ATOM	2042	OD2	ASP	A	269	49.333	-2.864	29.572	1.00	70.45	O
ATOM	2043	C	ASP	A	269	48.874	-3.700	32.336	1.00	55.85	C
ATOM	2044	O	ASP	A	269	48.867	-4.638	31.557	1.00	54.57	O
ATOM	2045	N	MET	A	270	47.995	-3.570	33.315	1.00	55.55	N
ATOM	2046	CA	MET	A	270	46.967	-4.547	33.602	1.00	56.02	C
ATOM	2047	CB	MET	A	270	45.732	-3.846	34.151	1.00	60.95	C
ATOM	2048	CG	MET	A	270	44.714	-4.808	34.734	1.00	63.95	C
ATOM	2049	SD	MET	A	270	45.502	-5.984	35.860	1.00	66.68	S
ATOM	2050	CE	MET	A	270	45.144	-5.216	37.467	1.00	65.33	C
ATOM	2051	C	MET	A	270	46.535	-5.523	32.529	1.00	55.88	C
ATOM	2052	O	MET	A	270	46.148	-6.644	32.853	1.00	57.92	O
ATOM	2053	N	TRP	A	271	46.573	-5.132	31.261	1.00	55.50	N
ATOM	2054	CA	TRP	A	271	46.140	-6.068	30.222	1.00	55.35	C
ATOM	2055	CB	TRP	A	271	44.825	-5.588	29.592	1.00	51.05	C
ATOM	2056	CG	TRP	A	271	43.778	-5.297	30.616	1.00	46.77	C
ATOM	2057	CD2	TRP	A	271	43.571	-4.049	31.271	1.00	44.24	C
ATOM	2058	CE2	TRP	A	271	42.546	-4.239	32.220	1.00	45.66	C
ATOM	2059	CE3	TRP	A	271	44.154	-2.784	31.144	1.00	42.21	C
ATOM	2060	CD1	TRP	A	271	42.889	-6.178	31.177	1.00	46.06	C
ATOM	2061	NE1	TRP	A	271	42.144	-5.547	32.144	1.00	43.10	N
ATOM	2062	CZ2	TRP	A	271	42.097	-3.209	33.039	1.00	47.03	C
ATOM	2063	CZ3	TRP	A	271	43.708	-1.768	31.948	1.00	42.69	C
ATOM	2064	CH2	TRP	A	271	42.688	-1.982	32.887	1.00	47.11	C
ATOM	2065	C	TRP	A	271	47.180	-6.301	29.137	1.00	55.50	C
ATOM	2066	O	TRP	A	271	47.113	-7.285	28.392	1.00	59.79	O
ATOM	2067	N	GLY	A	272	48.152	-5.413	29.044	1.00	50.57	N
ATOM	2068	CA	GLY	A	272	49.145	-5.606	28.019	1.00	50.51	C
ATOM	2069	C	GLY	A	272	48.600	-5.023	26.741	1.00	51.16	C
ATOM	2070	O	GLY	A	272	49.079	-5.337	25.642	1.00	54.25	O

327/396

Figure 3B-38

ATOM	2071	N	ARG	A	273	47.578	-4.183	26.899	1.00	46.51	N
ATOM	2072	CA	ARG	A	273	46.957	-3.505	25.783	1.00	42.27	C
ATOM	2073	CB	ARG	A	273	45.765	-2.685	26.261	1.00	41.74	C
ATOM	2074	CG	ARG	A	273	45.243	-1.707	25.223	1.00	38.31	C
ATOM	2075	CD	ARG	A	273	43.910	-1.077	25.588	1.00	33.58	C
ATOM	2076	NE	ARG	A	273	43.670	0.048	24.698	1.00	39.68	N
ATOM	2077	CZ	ARG	A	273	42.867	1.069	24.961	1.00	38.50	C
ATOM	2078	NH1	ARG	A	273	42.739	2.046	24.081	1.00	36.37	N
ATOM	2079	NH2	ARG	A	273	42.197	1.110	26.095	1.00	37.14	N
ATOM	2080	C	ARG	A	273	48.001	-2.589	25.182	1.00	43.75	C
ATOM	2081	O	ARG	A	273	48.020	-2.371	23.968	1.00	43.74	O
ATOM	2082	N	PHE	A	274	48.871	-2.065	26.049	1.00	44.68	N
ATOM	2083	CA	PHE	A	274	49.962	-1.171	25.662	1.00	48.00	C
ATOM	2084	CB	PHE	A	274	49.634	0.260	26.031	1.00	48.02	C
ATOM	2085	CG	PHE	A	274	48.417	0.780	25.374	1.00	53.48	C
ATOM	2086	CD1	PHE	A	274	47.272	1.031	26.110	1.00	56.47	C
ATOM	2087	CD2	PHE	A	274	48.407	1.031	24.017	1.00	56.71	C
ATOM	2088	CE1	PHE	A	274	46.140	1.525	25.509	1.00	56.57	C
ATOM	2089	CE2	PHE	A	274	47.275	1.526	23.404	1.00	58.82	C
ATOM	2090	CZ	PHE	A	274	46.140	1.774	24.154	1.00	59.75	C
ATOM	2091	C	PHE	A	274	51.279	-1.528	26.338	1.00	50.32	C
ATOM	2092	O	PHE	A	274	51.409	-1.380	27.554	1.00	54.51	O
ATOM	2093	N	TRP	A	275	52.255	-1.967	25.546	1.00	48.54	N
ATOM	2094	CA	TRP	A	275	53.580	-2.332	26.047	1.00	48.62	C
ATOM	2095	CB	TRP	A	275	54.288	-3.246	25.059	1.00	42.47	C
ATOM	2096	CG	TRP	A	275	53.568	-4.503	24.759	1.00	40.86	C
ATOM	2097	CD2	TRP	A	275	53.977	-5.492	23.823	1.00	34.01	C
ATOM	2098	CE2	TRP	A	275	53.029	-6.544	23.880	1.00	34.64	C
ATOM	2099	CE3	TRP	A	275	55.052	-5.593	22.941	1.00	27.95	C
ATOM	2100	CD1	TRP	A	275	52.402	-4.974	25.340	1.00	41.86	C
ATOM	2101	NE1	TRP	A	275	52.077	-6.206	24.810	1.00	37.50	N
ATOM	2102	CZ2	TRP	A	275	53.135	-7.674	23.086	1.00	28.81	C
ATOM	2103	CZ3	TRP	A	275	55.149	-6.703	22.159	1.00	28.83	C
ATOM	2104	CH2	TRP	A	275	54.194	-7.736	22.235	1.00	29.77	C
ATOM	2105	C	TRP	A	275	54.425	-1.080	26.188	1.00	52.01	C
ATOM	2106	O	TRP	A	275	55.652	-1.127	26.167	1.00	52.16	O
ATOM	2107	N	THR	A	276	53.771	0.054	26.331	1.00	56.70	N
ATOM	2108	CA	THR	A	276	54.507	1.298	26.410	1.00	61.41	C
ATOM	2109	CB	THR	A	276	53.525	2.498	26.303	1.00	62.75	C
ATOM	2110	OG1	THR	A	276	54.259	3.725	26.359	1.00	64.50	O
ATOM	2111	CG2	THR	A	276	52.486	2.449	27.417	1.00	66.15	C
ATOM	2112	C	THR	A	276	55.398	1.417	27.648	1.00	60.81	C
ATOM	2113	O	THR	A	276	56.406	2.121	27.633	1.00	60.61	O
ATOM	2114	N	ASN	A	277	55.048	0.715	28.715	1.00	59.40	N
ATOM	2115	CA	ASN	A	277	55.851	0.804	29.921	1.00	57.92	C
ATOM	2116	CB	ASN	A	277	54.958	0.607	31.142	1.00	57.07	C
ATOM	2117	CG	ASN	A	277	54.288	1.898	31.584	1.00	53.99	C
ATOM	2118	OD1	ASN	A	277	53.436	1.890	32.464	1.00	52.57	O
ATOM	2119	ND2	ASN	A	277	54.685	3.013	30.984	1.00	49.85	N
ATOM	2120	C	ASN	A	277	57.071	-0.129	29.966	1.00	57.24	C
ATOM	2121	O	ASN	A	277	57.943	0.022	30.824	1.00	59.13	O
ATOM	2122	N	LEU	A	278	57.135	-1.081	29.041	1.00	53.45	N
ATOM	2123	CA	LEU	A	278	58.269	-1.996	28.949	1.00	47.16	C
ATOM	2124	CB	LEU	A	278	57.921	-3.222	28.108	1.00	46.49	C
ATOM	2125	CG	LEU	A	278	57.175	-4.443	28.656	1.00	51.66	C
ATOM	2126	CD1	LEU	A	278	56.169	-4.013	29.707	1.00	53.53	C

328/396

Figure 3B-39

ATOM	2127	CD2	LEU	A	278	56.512	-5.202	27.501	1.00	43.23	C
ATOM	2128	C	LEU	A	278	59.313	-1.230	28.184	1.00	47.64	C
ATOM	2129	O	LEU	A	278	60.018	-1.813	27.382	1.00	48.91	O
ATOM	2130	N	TYR	A	279	59.404	0.077	28.391	1.00	49.15	N
ATOM	2131	CA	TYR	A	279	60.376	0.862	27.637	1.00	50.83	C
ATOM	2132	CB	TYR	A	279	59.927	2.322	27.488	1.00	43.81	C
ATOM	2133	CG	TYR	A	279	60.849	3.102	26.588	1.00	35.91	C
ATOM	2134	CD1	TYR	A	279	61.159	2.633	25.326	1.00	31.21	C
ATOM	2135	CE1	TYR	A	279	62.070	3.290	24.520	1.00	29.07	C
ATOM	2136	CD2	TYR	A	279	61.470	4.268	27.024	1.00	37.15	C
ATOM	2137	CE2	TYR	A	279	62.385	4.937	26.222	1.00	30.58	C
ATOM	2138	CZ	TYR	A	279	62.677	4.435	24.972	1.00	29.64	C
ATOM	2139	OH	TYR	A	279	63.575	5.077	24.161	1.00	33.90	O
ATOM	2140	C	TYR	A	279	61.766	0.826	28.240	1.00	55.71	C
ATOM	2141	O	TYR	A	279	62.754	0.706	27.510	1.00	59.01	O
ATOM	2142	N	SER	A	280	61.837	0.931	29.569	1.00	59.16	N
ATOM	2143	CA	SER	A	280	63.101	0.916	30.302	1.00	58.42	C
ATOM	2144	CB	SER	A	280	62.857	1.280	31.756	1.00	60.79	C
ATOM	2145	OG	SER	A	280	62.297	2.580	31.847	1.00	65.77	O
ATOM	2146	C	SER	A	280	63.750	-0.451	30.213	1.00	58.43	C
ATOM	2147	O	SER	A	280	64.963	-0.571	30.306	1.00	58.08	O
ATOM	2148	N	LEU	A	281	62.929	-1.475	30.021	1.00	58.80	N
ATOM	2149	CA	LEU	A	281	63.410	-2.843	29.881	1.00	61.22	C
ATOM	2150	CB	LEU	A	281	62.347	-3.838	30.350	1.00	55.92	C
ATOM	2151	CG	LEU	A	281	62.155	-3.928	31.857	1.00	56.15	C
ATOM	2152	CD1	LEU	A	281	62.134	-2.537	32.443	1.00	55.04	C
ATOM	2153	CD2	LEU	A	281	60.876	-4.686	32.171	1.00	55.97	C
ATOM	2154	C	LEU	A	281	63.758	-3.166	28.429	1.00	65.50	C
ATOM	2155	O	LEU	A	281	64.438	-4.166	28.160	1.00	69.13	O
ATOM	2156	N	THR	A	282	63.303	-2.325	27.496	1.00	66.38	N
ATOM	2157	CA	THR	A	282	63.540	-2.583	26.075	1.00	65.80	C
ATOM	2158	CB	THR	A	282	62.226	-2.970	25.347	1.00	66.02	C
ATOM	2159	OG1	THR	A	282	61.327	-1.861	25.380	1.00	65.20	O
ATOM	2160	CG2	THR	A	282	61.555	-4.185	26.021	1.00	64.81	C
ATOM	2161	C	THR	A	282	64.204	-1.489	25.253	1.00	65.24	C
ATOM	2162	O	THR	A	282	64.476	-1.708	24.072	1.00	64.54	O
ATOM	2163	N	VAL	A	283	64.458	-0.324	25.851	1.00	64.78	N
ATOM	2164	CA	VAL	A	283	65.115	0.764	25.124	1.00	64.86	C
ATOM	2165	CB	VAL	A	283	65.513	1.928	26.098	1.00	62.23	C
ATOM	2166	CG1	VAL	A	283	66.298	1.395	27.255	1.00	64.21	C
ATOM	2167	CG2	VAL	A	283	66.312	2.986	25.372	1.00	60.63	C
ATOM	2168	C	VAL	A	283	66.338	0.144	24.434	1.00	66.46	C
ATOM	2169	O	VAL	A	283	67.101	-0.581	25.059	1.00	68.05	O
ATOM	2170	N	PRO	A	284	66.527	0.405	23.129	1.00	69.72	N
ATOM	2171	CD	PRO	A	284	65.746	1.306	22.259	1.00	71.64	C
ATOM	2172	CA	PRO	A	284	67.666	-0.165	22.400	1.00	71.54	C
ATOM	2173	CB	PRO	A	284	67.278	0.068	20.940	1.00	72.57	C
ATOM	2174	CG	PRO	A	284	66.604	1.401	21.005	1.00	71.17	C
ATOM	2175	C	PRO	A	284	69.050	0.392	22.749	1.00	71.99	C
ATOM	2176	O	PRO	A	284	70.044	-0.328	22.668	1.00	71.36	O
ATOM	2177	N	PHE	A	285	69.110	1.667	23.126	1.00	73.02	N
ATOM	2178	CA	PHE	A	285	70.369	2.311	23.494	1.00	76.11	C
ATOM	2179	CB	PHE	A	285	70.882	3.202	22.356	1.00	76.92	C
ATOM	2180	CG	PHE	A	285	70.669	2.620	20.988	1.00	81.14	C
ATOM	2181	CD1	PHE	A	285	69.524	2.914	20.268	1.00	82.94	C
ATOM	2182	CD2	PHE	A	285	71.583	1.736	20.444	1.00	82.29	C

329/396

Figure 3B-40

ATOM	2183	CE1	PHE	A	285	69.295	2.334	19.033	1.00	84.12	C
ATOM	2184	CE2	PHE	A	285	71.359	1.154	19.209	1.00	83.79	C
ATOM	2185	CZ	PHE	A	285	70.213	1.452	18.504	1.00	83.64	C
ATOM	2186	C	PHE	A	285	70.090	3.164	24.722	1.00	79.03	C
ATOM	2187	O	PHE	A	285	70.231	4.392	24.681	1.00	78.84	O
ATOM	2188	N	GLY	A	286	69.699	2.492	25.807	1.00	80.96	N
ATOM	2189	CA	GLY	A	286	69.356	3.152	27.060	1.00	83.94	C
ATOM	2190	C	GLY	A	286	70.210	4.278	27.632	1.00	85.97	C
ATOM	2191	O	GLY	A	286	69.859	4.842	28.671	1.00	85.02	O
ATOM	2192	N	GLN	A	287	71.313	4.630	26.979	1.00	88.77	N
ATOM	2193	CA	GLN	A	287	72.166	5.688	27.504	1.00	91.06	C
ATOM	2194	CB	GLN	A	287	73.636	5.253	27.456	1.00	94.75	C
ATOM	2195	CG	GLN	A	287	74.103	4.799	26.103	1.00	98.78	C
ATOM	2196	CD	GLN	A	287	74.103	5.925	25.110	1.00	102.40	C
ATOM	2197	OE1	GLN	A	287	74.856	6.891	25.248	1.00	105.43	O
ATOM	2198	NE2	GLN	A	287	73.248	5.820	24.103	1.00	105.37	N
ATOM	2199	C	GLN	A	287	71.985	7.049	26.840	1.00	89.53	C
ATOM	2200	O	GLN	A	287	72.478	8.057	27.347	1.00	90.47	O
ATOM	2201	N	LYS	A	288	71.290	7.088	25.709	1.00	86.78	N
ATOM	2202	CA	LYS	A	288	71.040	8.365	25.051	1.00	84.54	C
ATOM	2203	CB	LYS	A	288	70.560	8.155	23.614	1.00	86.26	C
ATOM	2204	CG	LYS	A	288	71.652	7.792	22.622	1.00	85.64	C
ATOM	2205	CD	LYS	A	288	72.479	9.001	22.230	1.00	85.57	C
ATOM	2206	CE	LYS	A	288	73.731	8.582	21.470	1.00	86.72	C
ATOM	2207	NZ	LYS	A	288	73.428	7.730	20.287	1.00	85.47	N
ATOM	2208	C	LYS	A	288	69.947	9.043	25.868	1.00	83.44	C
ATOM	2209	O	LYS	A	288	69.230	8.386	26.624	1.00	83.08	O
ATOM	2210	N	PRO	A	289	69.803	10.365	25.727	1.00	81.73	N
ATOM	2211	CD	PRO	A	289	70.594	11.228	24.838	1.00	80.79	C
ATOM	2212	CA	PRO	A	289	68.796	11.146	26.451	1.00	81.58	C
ATOM	2213	CB	PRO	A	289	68.886	12.509	25.786	1.00	80.81	C
ATOM	2214	CG	PRO	A	289	70.342	12.592	25.426	1.00	81.36	C
ATOM	2215	C	PRO	A	289	67.394	10.549	26.363	1.00	82.66	C
ATOM	2216	O	PRO	A	289	66.766	10.581	25.303	1.00	82.45	O
ATOM	2217	N	ASN	A	290	66.914	10.014	27.489	1.00	83.07	N
ATOM	2218	CA	ASN	A	290	65.591	9.389	27.572	1.00	79.79	C
ATOM	2219	CB	ASN	A	290	65.129	9.246	29.042	1.00	78.84	C
ATOM	2220	CG	ASN	A	290	64.174	8.052	29.263	1.00	78.05	C
ATOM	2221	OD1	ASN	A	290	63.690	7.819	30.374	1.00	74.66	O
ATOM	2222	ND2	ASN	A	290	63.913	7.297	28.205	1.00	80.13	N
ATOM	2223	C	ASN	A	290	64.589	10.220	26.789	1.00	77.59	C
ATOM	2224	O	ASN	A	290	64.508	11.445	26.941	1.00	75.40	O
ATOM	2225	N	ILE	A	291	63.848	9.529	25.930	1.00	75.36	N
ATOM	2226	CA	ILE	A	291	62.836	10.145	25.096	1.00	72.24	C
ATOM	2227	CB	ILE	A	291	62.948	9.628	23.647	1.00	69.97	C
ATOM	2228	CG2	ILE	A	291	62.104	8.374	23.446	1.00	66.01	C
ATOM	2229	CG1	ILE	A	291	62.550	10.750	22.703	1.00	69.95	C
ATOM	2230	CD1	ILE	A	291	63.257	12.043	23.030	1.00	67.11	C
ATOM	2231	C	ILE	A	291	61.454	9.844	25.682	1.00	71.98	C
ATOM	2232	O	ILE	A	291	60.433	9.904	24.990	1.00	72.80	O
ATOM	2233	N	ASP	A	292	61.453	9.505	26.971	1.00	68.94	N
ATOM	2234	CA	ASP	A	292	60.242	9.223	27.732	1.00	66.82	C
ATOM	2235	CB	ASP	A	292	60.331	7.843	28.404	1.00	67.00	C
ATOM	2236	CG	ASP	A	292	59.162	7.558	29.351	1.00	67.02	C
ATOM	2237	OD1	ASP	A	292	59.065	6.420	29.859	1.00	69.77	O
ATOM	2238	OD2	ASP	A	292	58.343	8.459	29.605	1.00	66.26	O

330/396

Figure 3B-41

ATOM	2239	C	ASP	A	292	60.208	10.338	28.775	1.00	66.40	C
ATOM	2240	O	ASP	A	292	60.399	10.107	29.973	1.00	67.27	O
ATOM	2241	N	VAL	A	293	59.982	11.555	28.283	1.00	64.14	N
ATOM	2242	CA	VAL	A	293	59.919	12.768	29.088	1.00	63.91	C
ATOM	2243	CB	VAL	A	293	59.494	13.945	28.220	1.00	61.74	C
ATOM	2244	CG1	VAL	A	293	60.416	14.059	27.036	1.00	61.41	C
ATOM	2245	CG2	VAL	A	293	58.077	13.742	27.749	1.00	63.24	C
ATOM	2246	C	VAL	A	293	58.966	12.683	30.277	1.00	66.85	C
ATOM	2247	O	VAL	A	293	58.357	13.684	30.678	1.00	66.58	O
ATOM	2248	N	THR	A	294	58.838	11.485	30.838	1.00	67.39	N
ATOM	2249	CA	THR	A	294	57.970	11.262	31.979	1.00	68.27	C
ATOM	2250	CB	THR	A	294	57.720	9.760	32.200	1.00	68.09	C
ATOM	2251	OG1	THR	A	294	56.932	9.572	33.379	1.00	67.91	O
ATOM	2252	CG2	THR	A	294	59.026	9.029	32.358	1.00	69.88	C
ATOM	2253	C	THR	A	294	58.682	11.834	33.178	1.00	67.98	C
ATOM	2254	O	THR	A	294	58.059	12.361	34.089	1.00	65.28	O
ATOM	2255	N	ASP	A	295	60.007	11.744	33.137	1.00	72.19	N
ATOM	2256	CA	ASP	A	295	60.882	12.229	34.205	1.00	75.46	C
ATOM	2257	CB	ASP	A	295	62.219	11.475	34.134	1.00	76.65	C
ATOM	2258	CG	ASP	A	295	62.032	9.962	33.948	1.00	79.11	C
ATOM	2259	OD1	ASP	A	295	61.863	9.246	34.963	1.00	76.49	O
ATOM	2260	OD2	ASP	A	295	62.036	9.493	32.780	1.00	76.70	O
ATOM	2261	C	ASP	A	295	61.109	13.742	34.088	1.00	75.17	C
ATOM	2262	O	ASP	A	295	60.924	14.488	35.047	1.00	75.85	O
ATOM	2263	N	ALA	A	296	61.505	14.190	32.904	1.00	76.52	N
ATOM	2264	CA	ALA	A	296	61.740	15.605	32.668	1.00	77.40	C
ATOM	2265	CB	ALA	A	296	61.993	15.840	31.190	1.00	76.80	C
ATOM	2266	C	ALA	A	296	60.540	16.423	33.125	1.00	78.79	C
ATOM	2267	O	ALA	A	296	60.670	17.590	33.479	1.00	77.94	O
ATOM	2268	N	MET	A	297	59.368	15.796	33.114	1.00	82.06	N
ATOM	2269	CA	MET	A	297	58.125	16.455	33.510	1.00	84.53	C
ATOM	2270	CB	MET	A	297	56.918	15.606	33.082	1.00	85.00	C
ATOM	2271	CG	MET	A	297	56.595	15.645	31.591	1.00	82.18	C
ATOM	2272	SD	MET	A	297	55.207	14.579	31.166	1.00	78.30	S
ATOM	2273	CE	MET	A	297	53.843	15.506	31.847	1.00	73.93	C
ATOM	2274	C	MET	A	297	58.056	16.710	35.008	1.00	85.38	C
ATOM	2275	O	MET	A	297	57.528	17.734	35.453	1.00	84.93	O
ATOM	2276	N	VAL	A	298	58.581	15.766	35.783	1.00	86.70	N
ATOM	2277	CA	VAL	A	298	58.584	15.881	37.234	1.00	86.61	C
ATOM	2278	CB	VAL	A	298	58.880	14.521	37.899	1.00	85.07	C
ATOM	2279	CG1	VAL	A	298	58.653	14.621	39.396	1.00	86.94	C
ATOM	2280	CG2	VAL	A	298	57.995	13.446	37.303	1.00	81.95	C
ATOM	2281	C	VAL	A	298	59.642	16.901	37.661	1.00	87.50	C
ATOM	2282	O	VAL	A	298	59.372	17.772	38.493	1.00	86.68	O
ATOM	2283	N	ASP	A	299	60.839	16.795	37.084	1.00	87.44	N
ATOM	2284	CA	ASP	A	299	61.919	17.727	37.397	1.00	87.73	C
ATOM	2285	CB	ASP	A	299	63.263	17.219	36.867	1.00	90.96	C
ATOM	2286	CG	ASP	A	299	63.835	16.090	37.702	1.00	95.14	C
ATOM	2287	OD1	ASP	A	299	63.687	16.132	38.944	1.00	97.10	O
ATOM	2288	OD2	ASP	A	299	64.452	15.170	37.119	1.00	96.67	O
ATOM	2289	C	ASP	A	299	61.629	19.083	36.774	1.00	86.36	C
ATOM	2290	O	ASP	A	299	62.539	19.754	36.290	1.00	87.06	O
ATOM	2291	N	GLN	A	300	60.355	19.465	36.776	1.00	83.65	N
ATOM	2292	CA	GLN	A	300	59.895	20.736	36.226	1.00	80.22	C
ATOM	2293	CB	GLN	A	300	59.697	20.617	34.706	1.00	76.92	C
ATOM	2294	CG	GLN	A	300	60.119	21.857	33.913	1.00	74.34	C

331/396

Figure 3B-42

ATOM	2295	CD	GLN	A	300	60.425	21.567	32.437	1.00	75.45	C
ATOM	2296	OE1	GLN	A	300	61.275	20.732	32.112	1.00	74.11	O
ATOM	2297	NE2	GLN	A	300	59.740	22.270	31.543	1.00	73.70	N
ATOM	2298	C	GLN	A	300	58.572	20.979	36.940	1.00	79.95	C
ATOM	2299	O	GLN	A	300	57.955	22.037	36.825	1.00	77.44	O
ATOM	2300	N	ALA	A	301	58.164	19.968	37.699	1.00	81.56	N
ATOM	2301	CA	ALA	A	301	56.936	20.003	38.473	1.00	84.83	C
ATOM	2302	CB	ALA	A	301	57.040	21.042	39.562	1.00	83.48	C
ATOM	2303	C	ALA	A	301	55.726	20.286	37.609	1.00	88.21	C
ATOM	2304	O	ALA	A	301	54.945	21.184	37.907	1.00	88.61	O
ATOM	2305	N	TRP	A	302	55.575	19.520	36.535	1.00	92.14	N
ATOM	2306	CA	TRP	A	302	54.443	19.690	35.631	1.00	94.75	C
ATOM	2307	CB	TRP	A	302	54.644	18.869	34.358	1.00	100.30	C
ATOM	2308	CG	TRP	A	302	55.335	19.569	33.244	1.00	106.33	C
ATOM	2309	CD2	TRP	A	302	54.785	19.866	31.956	1.00	109.03	C
ATOM	2310	CE2	TRP	A	302	55.803	20.479	31.199	1.00	110.81	C
ATOM	2311	CE3	TRP	A	302	53.532	19.672	31.369	1.00	109.70	C
ATOM	2312	CD1	TRP	A	302	56.624	20.007	33.221	1.00	109.68	C
ATOM	2313	NE1	TRP	A	302	56.916	20.555	31.993	1.00	111.64	N
ATOM	2314	CZ2	TRP	A	302	55.605	20.899	29.886	1.00	111.08	C
ATOM	2315	CZ3	TRP	A	302	53.337	20.090	30.069	1.00	110.66	C
ATOM	2316	CH2	TRP	A	302	54.369	20.697	29.341	1.00	111.70	C
ATOM	2317	C	TRP	A	302	53.187	19.186	36.316	1.00	93.75	C
ATOM	2318	O	TRP	A	302	53.223	18.152	36.977	1.00	93.54	O
ATOM	2319	N	ASP	A	303	52.077	19.901	36.157	1.00	92.08	N
ATOM	2320	CA	ASP	A	303	50.822	19.456	36.757	1.00	91.33	C
ATOM	2321	CB	ASP	A	303	50.347	20.446	37.823	1.00	89.11	C
ATOM	2322	CG	ASP	A	303	50.197	21.840	37.290	1.00	88.51	C
ATOM	2323	OD1	ASP	A	303	49.611	22.686	37.998	1.00	88.96	O
ATOM	2324	OD2	ASP	A	303	50.674	22.088	36.166	1.00	87.44	O
ATOM	2325	C	ASP	A	303	49.708	19.228	35.722	1.00	91.03	C
ATOM	2326	O	ASP	A	303	49.942	19.266	34.508	1.00	89.38	O
ATOM	2327	N	ALA	A	304	48.499	18.974	36.215	1.00	89.60	N
ATOM	2328	CA	ALA	A	304	47.359	18.729	35.347	1.00	86.06	C
ATOM	2329	CB	ALA	A	304	46.088	18.608	36.174	1.00	86.54	C
ATOM	2330	C	ALA	A	304	47.233	19.862	34.347	1.00	84.88	C
ATOM	2331	O	ALA	A	304	47.593	19.705	33.182	1.00	85.10	O
ATOM	2332	N	GLN	A	305	46.735	21.006	34.809	1.00	82.93	N
ATOM	2333	CA	GLN	A	305	46.558	22.168	33.947	1.00	81.71	C
ATOM	2334	CB	GLN	A	305	46.456	23.441	34.788	1.00	85.70	C
ATOM	2335	CG	GLN	A	305	46.321	24.722	33.974	1.00	93.26	C
ATOM	2336	CD	GLN	A	305	45.161	25.601	34.439	1.00	98.37	C
ATOM	2337	OE1	GLN	A	305	43.990	25.214	34.339	1.00	99.83	O
ATOM	2338	NE2	GLN	A	305	45.483	26.792	34.947	1.00	98.80	N
ATOM	2339	C	GLN	A	305	47.704	22.291	32.953	1.00	78.63	C
ATOM	2340	O	GLN	A	305	47.526	22.053	31.766	1.00	78.21	O
ATOM	2341	N	ARG	A	306	48.883	22.651	33.443	1.00	76.49	N
ATOM	2342	CA	ARG	A	306	50.055	22.800	32.592	1.00	71.62	C
ATOM	2343	CB	ARG	A	306	51.320	22.549	33.398	1.00	69.47	C
ATOM	2344	CG	ARG	A	306	52.574	22.531	32.561	1.00	71.01	C
ATOM	2345	CD	ARG	A	306	52.904	23.907	32.046	1.00	72.14	C
ATOM	2346	NE	ARG	A	306	54.075	23.910	31.172	1.00	74.61	N
ATOM	2347	CZ	ARG	A	306	55.285	23.484	31.523	1.00	75.64	C
ATOM	2348	NH1	ARG	A	306	55.506	23.008	32.741	1.00	76.06	N
ATOM	2349	NH2	ARG	A	306	56.281	23.538	30.649	1.00	76.83	N
ATOM	2350	C	ARG	A	306	50.024	21.848	31.408	1.00	70.42	C

332/396

Figure 3B-43

ATOM	2351	O	ARG	A	306	50.343	22.239	30.288	1.00	71.19	O
ATOM	2352	N	ILE	A	307	49.637	20.599	31.662	1.00	69.84	N
ATOM	2353	CA	ILE	A	307	49.570	19.576	30.616	1.00	68.70	C
ATOM	2354	CB	ILE	A	307	49.283	18.178	31.206	1.00	66.32	C
ATOM	2355	CG2	ILE	A	307	48.885	17.231	30.107	1.00	65.87	C
ATOM	2356	CG1	ILE	A	307	50.518	17.648	31.935	1.00	63.52	C
ATOM	2357	CD1	ILE	A	307	50.361	16.238	32.450	1.00	59.12	C
ATOM	2358	C	ILE	A	307	48.495	19.893	29.589	1.00	68.96	C
ATOM	2359	O	ILE	A	307	48.790	20.123	28.419	1.00	68.66	O
ATOM	2360	N	PHE	A	308	47.245	19.899	30.032	1.00	69.40	N
ATOM	2361	CA	PHE	A	308	46.126	20.204	29.153	1.00	69.64	C
ATOM	2362	CB	PHE	A	308	44.816	20.093	29.932	1.00	67.13	C
ATOM	2363	CG	PHE	A	308	44.304	18.695	30.040	1.00	66.97	C
ATOM	2364	CD1	PHE	A	308	43.568	18.137	29.014	1.00	65.75	C
ATOM	2365	CD2	PHE	A	308	44.596	17.922	31.142	1.00	66.38	C
ATOM	2366	CE1	PHE	A	308	43.135	16.835	29.084	1.00	65.85	C
ATOM	2367	CE2	PHE	A	308	44.163	16.617	31.213	1.00	67.46	C
ATOM	2368	CZ	PHE	A	308	43.433	16.073	30.181	1.00	65.89	C
ATOM	2369	C	PHE	A	308	46.256	21.595	28.547	1.00	70.89	C
ATOM	2370	O	PHE	A	308	45.610	21.911	27.555	1.00	73.64	O
ATOM	2371	N	LYS	A	309	47.096	22.426	29.148	1.00	72.32	N
ATOM	2372	CA	LYS	A	309	47.299	23.777	28.655	1.00	73.21	C
ATOM	2373	CB	LYS	A	309	47.839	24.671	29.770	1.00	72.20	C
ATOM	2374	CG	LYS	A	309	47.439	26.133	29.658	1.00	71.47	C
ATOM	2375	CD	LYS	A	309	45.978	26.362	30.033	1.00	68.57	C
ATOM	2376	CE	LYS	A	309	45.607	27.833	29.894	1.00	68.16	C
ATOM	2377	NZ	LYS	A	309	44.234	28.140	30.381	1.00	69.10	N
ATOM	2378	C	LYS	A	309	48.312	23.679	27.533	1.00	74.53	C
ATOM	2379	O	LYS	A	309	48.221	24.377	26.527	1.00	74.91	O
ATOM	2380	N	GLU	A	310	49.279	22.791	27.714	1.00	78.16	N
ATOM	2381	CA	GLU	A	310	50.315	22.586	26.714	1.00	82.74	C
ATOM	2382	CB	GLU	A	310	51.501	21.834	27.326	1.00	86.35	C
ATOM	2383	CG	GLU	A	310	52.796	21.949	26.528	1.00	92.11	C
ATOM	2384	CD	GLU	A	310	53.508	23.270	26.768	1.00	96.52	C
ATOM	2385	OE1	GLU	A	310	53.897	23.531	27.927	1.00	100.04	O
ATOM	2386	OE2	GLU	A	310	53.680	24.050	25.808	1.00	97.94	O
ATOM	2387	C	GLU	A	310	49.746	21.779	25.541	1.00	82.85	C
ATOM	2388	O	GLU	A	310	50.305	21.789	24.443	1.00	84.48	O
ATOM	2389	N	ALA	A	311	48.641	21.075	25.780	1.00	80.86	N
ATOM	2390	CA	ALA	A	311	48.002	20.269	24.741	1.00	77.14	C
ATOM	2391	CB	ALA	A	311	47.192	19.141	25.374	1.00	77.88	C
ATOM	2392	C	ALA	A	311	47.101	21.168	23.908	1.00	75.20	C
ATOM	2393	O	ALA	A	311	47.195	21.193	22.682	1.00	74.15	O
ATOM	2394	N	GLU	A	312	46.229	21.903	24.592	1.00	72.72	N
ATOM	2395	CA	GLU	A	312	45.319	22.838	23.948	1.00	73.16	C
ATOM	2396	CB	GLU	A	312	44.531	23.594	25.008	1.00	72.44	C
ATOM	2397	CG	GLU	A	312	43.767	24.793	24.494	1.00	70.19	C
ATOM	2398	CD	GLU	A	312	43.611	25.845	25.567	1.00	69.84	C
ATOM	2399	OE1	GLU	A	312	44.662	26.283	26.086	1.00	69.05	O
ATOM	2400	OE2	GLU	A	312	42.460	26.230	25.892	1.00	65.64	O
ATOM	2401	C	GLU	A	312	46.137	23.826	23.126	1.00	74.32	C
ATOM	2402	O	GLU	A	312	45.674	24.365	22.118	1.00	74.40	O
ATOM	2403	N	LYS	A	313	47.359	24.068	23.577	1.00	75.23	N
ATOM	2404	CA	LYS	A	313	48.260	24.972	22.883	1.00	75.95	C
ATOM	2405	CB	LYS	A	313	49.527	25.192	23.718	1.00	76.24	C
ATOM	2406	CG	LYS	A	313	50.668	25.864	22.964	1.00	78.77	C

333/396

Figure 3B-44

ATOM	2407	CD	LYS	A	313	50.270	27.249	22.463	1.00	83.10	C
ATOM	2408	CE	LYS	A	313	51.341	27.860	21.560	1.00	81.21	C
ATOM	2409	NZ	LYS	A	313	51.511	27.099	20.289	1.00	80.70	N
ATOM	2410	C	LYS	A	313	48.627	24.389	21.522	1.00	75.15	C
ATOM	2411	O	LYS	A	313	48.981	25.117	20.603	1.00	73.95	O
ATOM	2412	N	PHE	A	314	48.535	23.071	21.394	1.00	76.54	N
ATOM	2413	CA	PHE	A	314	48.880	22.411	20.142	1.00	78.16	C
ATOM	2414	CB	PHE	A	314	49.049	20.910	20.369	1.00	78.77	C
ATOM	2415	CG	PHE	A	314	49.784	20.214	19.263	1.00	82.76	C
ATOM	2416	CD1	PHE	A	314	51.147	19.995	19.351	1.00	85.50	C
ATOM	2417	CD2	PHE	A	314	49.118	19.800	18.120	1.00	84.01	C
ATOM	2418	CE1	PHE	A	314	51.834	19.374	18.316	1.00	87.51	C
ATOM	2419	CE2	PHE	A	314	49.800	19.180	17.081	1.00	85.75	C
ATOM	2420	CZ	PHE	A	314	51.157	18.967	17.179	1.00	87.18	C
ATOM	2421	C	PHE	A	314	47.833	22.652	19.047	1.00	78.19	C
ATOM	2422	O	PHE	A	314	48.165	23.064	17.939	1.00	77.16	O
ATOM	2423	N	PHE	A	315	46.571	22.390	19.359	1.00	78.32	N
ATOM	2424	CA	PHE	A	315	45.494	22.581	18.395	1.00	79.57	C
ATOM	2425	CB	PHE	A	315	44.172	22.159	19.027	1.00	80.69	C
ATOM	2426	CG	PHE	A	315	44.109	20.701	19.350	1.00	84.76	C
ATOM	2427	CD1	PHE	A	315	43.846	19.771	18.358	1.00	85.09	C
ATOM	2428	CD2	PHE	A	315	44.363	20.250	20.639	1.00	87.50	C
ATOM	2429	CE1	PHE	A	315	43.838	18.416	18.642	1.00	87.53	C
ATOM	2430	CE2	PHE	A	315	44.358	18.894	20.934	1.00	88.58	C
ATOM	2431	CZ	PHE	A	315	44.095	17.976	19.933	1.00	89.38	C
ATOM	2432	C	PHE	A	315	45.406	24.022	17.901	1.00	79.85	C
ATOM	2433	O	PHE	A	315	45.146	24.282	16.721	1.00	79.97	O
ATOM	2434	N	VAL	A	316	45.627	24.962	18.809	1.00	79.19	N
ATOM	2435	CA	VAL	A	316	45.575	26.372	18.463	1.00	77.87	C
ATOM	2436	CB	VAL	A	316	45.597	27.239	19.747	1.00	78.92	C
ATOM	2437	CG1	VAL	A	316	46.902	27.040	20.489	1.00	78.09	C
ATOM	2438	CG2	VAL	A	316	45.390	28.697	19.400	1.00	81.03	C
ATOM	2439	C	VAL	A	316	46.738	26.763	17.545	1.00	75.77	C
ATOM	2440	O	VAL	A	316	46.728	27.821	16.928	1.00	73.87	O
ATOM	2441	N	SER	A	317	47.738	25.896	17.443	1.00	76.02	N
ATOM	2442	CA	SER	A	317	48.888	26.187	16.603	1.00	76.50	C
ATOM	2443	CB	SER	A	317	50.136	25.472	17.124	1.00	75.82	C
ATOM	2444	OG	SER	A	317	50.156	24.117	16.723	1.00	72.97	O
ATOM	2445	C	SER	A	317	48.624	25.764	15.168	1.00	77.98	C
ATOM	2446	O	SER	A	317	49.427	26.035	14.277	1.00	79.12	O
ATOM	2447	N	VAL	A	318	47.501	25.090	14.945	1.00	78.19	N
ATOM	2448	CA	VAL	A	318	47.138	24.655	13.601	1.00	78.64	C
ATOM	2449	CB	VAL	A	318	47.390	23.147	13.398	1.00	76.08	C
ATOM	2450	CG1	VAL	A	318	48.870	22.857	13.480	1.00	74.63	C
ATOM	2451	CG2	VAL	A	318	46.640	22.351	14.437	1.00	75.04	C
ATOM	2452	C	VAL	A	318	45.670	24.955	13.325	1.00	80.36	C
ATOM	2453	O	VAL	A	318	44.909	24.082	12.915	1.00	82.12	O
ATOM	2454	N	GLY	A	319	45.278	26.203	13.553	1.00	79.27	N
ATOM	2455	CA	GLY	A	319	43.907	26.594	13.318	1.00	78.76	C
ATOM	2456	C	GLY	A	319	43.053	26.403	14.548	1.00	79.97	C
ATOM	2457	O	GLY	A	319	43.024	27.262	15.422	1.00	80.76	O
ATOM	2458	N	LEU	A	320	42.370	25.264	14.607	1.00	81.42	N
ATOM	2459	CA	LEU	A	320	41.472	24.901	15.702	1.00	81.11	C
ATOM	2460	CB	LEU	A	320	41.710	23.448	16.110	1.00	82.53	C
ATOM	2461	CG	LEU	A	320	41.346	22.410	15.045	1.00	83.00	C
ATOM	2462	CD1	LEU	A	320	39.877	22.544	14.660	1.00	85.50	C

334/396

Figure 3B-45

ATOM	2463	CD2	LEU	A	320	42.224	22.609	13.829	1.00	83.50	C
ATOM	2464	C	LEU	A	320	41.531	25.802	16.926	1.00	81.06	C
ATOM	2465	O	LEU	A	320	42.604	26.122	17.434	1.00	80.87	O
ATOM	2466	N	PRO	A	321	40.358	26.206	17.426	1.00	81.60	N
ATOM	2467	CD	PRO	A	321	39.062	25.692	16.950	1.00	80.25	C
ATOM	2468	CA	PRO	A	321	40.175	27.079	18.589	1.00	84.84	C
ATOM	2469	CB	PRO	A	321	38.652	27.179	18.698	1.00	82.12	C
ATOM	2470	CG	PRO	A	321	38.188	25.869	18.154	1.00	79.65	C
ATOM	2471	C	PRO	A	321	40.828	26.619	19.894	1.00	88.36	C
ATOM	2472	O	PRO	A	321	41.562	25.629	19.927	1.00	90.35	O
ATOM	2473	N	ASN	A	322	40.568	27.366	20.965	1.00	90.74	N
ATOM	2474	CA	ASN	A	322	41.096	27.037	22.284	1.00	91.99	C
ATOM	2475	CB	ASN	A	322	41.594	28.293	23.007	1.00	96.66	C
ATOM	2476	CG	ASN	A	322	42.496	29.152	22.139	1.00	101.79	C
ATOM	2477	OD1	ASN	A	322	43.398	28.641	21.471	1.00	103.75	O
ATOM	2478	ND2	ASN	A	322	42.265	30.468	22.153	1.00	102.49	N
ATOM	2479	C	ASN	A	322	39.930	26.448	23.059	1.00	90.29	C
ATOM	2480	O	ASN	A	322	38.777	26.738	22.753	1.00	88.96	O
ATOM	2481	N	MET	A	323	40.218	25.619	24.054	1.00	89.88	N
ATOM	2482	CA	MET	A	323	39.148	25.026	24.843	1.00	88.88	C
ATOM	2483	CB	MET	A	323	39.719	24.221	26.007	1.00	88.28	C
ATOM	2484	CG	MET	A	323	40.537	23.026	25.590	1.00	86.55	C
ATOM	2485	SD	MET	A	323	39.583	21.921	24.558	1.00	85.62	S
ATOM	2486	CE	MET	A	323	40.297	22.281	22.981	1.00	86.21	C
ATOM	2487	C	MET	A	323	38.273	26.145	25.380	1.00	88.60	C
ATOM	2488	O	MET	A	323	38.781	27.184	25.806	1.00	88.01	O
ATOM	2489	N	THR	A	324	36.960	25.936	25.351	1.00	88.01	N
ATOM	2490	CA	THR	A	324	36.022	26.939	25.838	1.00	88.14	C
ATOM	2491	CB	THR	A	324	34.558	26.525	25.580	1.00	87.23	C
ATOM	2492	OG1	THR	A	324	34.221	25.389	26.386	1.00	85.66	O
ATOM	2493	CG2	THR	A	324	34.363	26.176	24.122	1.00	86.44	C
ATOM	2494	C	THR	A	324	36.207	27.142	27.334	1.00	89.19	C
ATOM	2495	O	THR	A	324	36.549	26.207	28.058	1.00	90.29	O
ATOM	2496	N	GLN	A	325	35.987	28.368	27.794	1.00	88.42	N
ATOM	2497	CA	GLN	A	325	36.128	28.672	29.208	1.00	88.01	C
ATOM	2498	CB	GLN	A	325	35.872	30.160	29.441	1.00	88.18	C
ATOM	2499	CG	GLN	A	325	35.716	30.552	30.888	1.00	91.33	C
ATOM	2500	CD	GLN	A	325	35.529	32.043	31.058	1.00	94.80	C
ATOM	2501	OE1	GLN	A	325	36.481	32.816	30.937	1.00	96.61	O
ATOM	2502	NE2	GLN	A	325	34.293	32.460	31.327	1.00	94.87	N
ATOM	2503	C	GLN	A	325	35.162	27.814	30.029	1.00	87.74	C
ATOM	2504	O	GLN	A	325	35.325	27.669	31.238	1.00	89.86	O
ATOM	2505	N	GLY	A	326	34.158	27.240	29.368	1.00	86.27	N
ATOM	2506	CA	GLY	A	326	33.209	26.382	30.060	1.00	83.09	C
ATOM	2507	C	GLY	A	326	33.875	25.045	30.325	1.00	82.06	C
ATOM	2508	O	GLY	A	326	33.650	24.404	31.347	1.00	79.47	O
ATOM	2509	N	PHE	A	327	34.707	24.625	29.380	1.00	81.97	N
ATOM	2510	CA	PHE	A	327	35.446	23.379	29.500	1.00	82.96	C
ATOM	2511	CB	PHE	A	327	36.253	23.133	28.219	1.00	85.38	C
ATOM	2512	CG	PHE	A	327	37.373	22.130	28.371	1.00	87.09	C
ATOM	2513	CD1	PHE	A	327	38.608	22.514	28.870	1.00	84.40	C
ATOM	2514	CD2	PHE	A	327	37.196	20.808	27.989	1.00	88.62	C
ATOM	2515	CE1	PHE	A	327	39.640	21.607	28.984	1.00	84.05	C
ATOM	2516	CE2	PHE	A	327	38.229	19.895	28.103	1.00	87.74	C
ATOM	2517	CZ	PHE	A	327	39.452	20.297	28.601	1.00	85.78	C
ATOM	2518	C	PHE	A	327	36.377	23.480	30.699	1.00	82.92	C

335/396

Figure 3B-46

ATOM	2519	O	PHE	A	327	36.357	22.627	31.587	1.00	83.04	O
ATOM	2520	N	TRP	A	328	37.185	24.539	30.719	1.00	81.96	N
ATOM	2521	CA	TRP	A	328	38.137	24.770	31.797	1.00	80.02	C
ATOM	2522	CB	TRP	A	328	38.917	26.061	31.558	1.00	78.33	C
ATOM	2523	CG	TRP	A	328	40.078	25.898	30.641	1.00	79.10	C
ATOM	2524	CD2	TRP	A	328	41.252	25.117	30.877	1.00	78.01	C
ATOM	2525	CE2	TRP	A	328	42.067	25.232	29.732	1.00	79.41	C
ATOM	2526	CE3	TRP	A	328	41.693	24.332	31.943	1.00	79.64	C
ATOM	2527	CD1	TRP	A	328	40.225	26.443	29.402	1.00	81.44	C
ATOM	2528	NE1	TRP	A	328	41.420	26.048	28.846	1.00	80.16	N
ATOM	2529	CZ2	TRP	A	328	43.297	24.590	29.622	1.00	81.82	C
ATOM	2530	CZ3	TRP	A	328	42.914	23.696	31.837	1.00	82.56	C
ATOM	2531	CH2	TRP	A	328	43.704	23.829	30.681	1.00	84.60	C
ATOM	2532	C	TRP	A	328	37.498	24.841	33.170	1.00	80.42	C
ATOM	2533	O	TRP	A	328	38.188	24.694	34.175	1.00	80.54	O
ATOM	2534	N	GLU	A	329	36.186	25.047	33.219	1.00	80.58	N
ATOM	2535	CA	GLU	A	329	35.503	25.162	34.499	1.00	80.38	C
ATOM	2536	CB	GLU	A	329	34.694	26.459	34.517	1.00	82.42	C
ATOM	2537	CG	GLU	A	329	34.174	26.846	35.888	1.00	88.65	C
ATOM	2538	CD	GLU	A	329	33.634	28.262	35.932	1.00	92.23	C
ATOM	2539	OE1	GLU	A	329	32.626	28.543	35.243	1.00	94.18	O
ATOM	2540	OE2	GLU	A	329	34.225	29.094	36.658	1.00	92.40	O
ATOM	2541	C	GLU	A	329	34.620	23.983	34.940	1.00	79.61	C
ATOM	2542	O	GLU	A	329	33.827	24.119	35.870	1.00	80.91	O
ATOM	2543	N	ASN	A	330	34.739	22.827	34.290	1.00	76.12	N
ATOM	2544	CA	ASN	A	330	33.950	21.667	34.710	1.00	71.88	C
ATOM	2545	CB	ASN	A	330	32.638	21.584	33.947	1.00	70.70	C
ATOM	2546	CG	ASN	A	330	31.935	22.898	33.883	1.00	71.05	C
ATOM	2547	OD1	ASN	A	330	32.280	23.755	33.076	1.00	70.17	O
ATOM	2548	ND2	ASN	A	330	30.953	23.084	34.748	1.00	72.21	N
ATOM	2549	C	ASN	A	330	34.723	20.382	34.496	1.00	70.60	C
ATOM	2550	O	ASN	A	330	34.456	19.366	35.136	1.00	69.75	O
ATOM	2551	N	SER	A	331	35.685	20.418	33.588	1.00	68.12	N
ATOM	2552	CA	SER	A	331	36.467	19.228	33.330	1.00	67.28	C
ATOM	2553	CB	SER	A	331	37.513	19.496	32.245	1.00	66.94	C
ATOM	2554	OG	SER	A	331	36.910	19.839	31.009	1.00	66.19	O
ATOM	2555	C	SER	A	331	37.158	18.837	34.622	1.00	66.94	C
ATOM	2556	O	SER	A	331	37.730	19.689	35.299	1.00	68.05	O
ATOM	2557	N	MET	A	332	37.077	17.556	34.973	1.00	67.03	N
ATOM	2558	CA	MET	A	332	37.735	17.027	36.169	1.00	65.01	C
ATOM	2559	CB	MET	A	332	36.867	15.950	36.808	1.00	59.63	C
ATOM	2560	CG	MET	A	332	37.469	15.331	38.030	1.00	59.79	C
ATOM	2561	SD	MET	A	332	36.259	14.339	38.898	1.00	63.72	S
ATOM	2562	CE	MET	A	332	35.923	15.376	40.286	1.00	64.87	C
ATOM	2563	C	MET	A	332	39.052	16.429	35.678	1.00	66.35	C
ATOM	2564	O	MET	A	332	39.071	15.314	35.162	1.00	68.24	O
ATOM	2565	N	LEU	A	333	40.147	17.171	35.833	1.00	67.03	N
ATOM	2566	CA	LEU	A	333	41.459	16.734	35.349	1.00	69.64	C
ATOM	2567	CB	LEU	A	333	42.155	17.919	34.675	1.00	67.18	C
ATOM	2568	CG	LEU	A	333	41.314	18.765	33.715	1.00	65.42	C
ATOM	2569	CD1	LEU	A	333	42.165	19.883	33.147	1.00	66.02	C
ATOM	2570	CD2	LEU	A	333	40.770	17.908	32.601	1.00	66.84	C
ATOM	2571	C	LEU	A	333	42.424	16.087	36.365	1.00	73.86	C
ATOM	2572	O	LEU	A	333	43.639	16.049	36.135	1.00	72.22	O
ATOM	2573	N	THR	A	334	41.879	15.575	37.469	1.00	77.89	N
ATOM	2574	CA	THR	A	334	42.651	14.916	38.531	1.00	80.47	C

336/396

Figure 3B-47

ATOM	2575	CB	THR	A	334	43.517	15.904	39.330	1.00	79.39	C
ATOM	2576	OG1	THR	A	334	42.790	17.125	39.528	1.00	75.56	O
ATOM	2577	CG2	THR	A	334	44.832	16.173	38.618	1.00	80.21	C
ATOM	2578	C	THR	A	334	41.693	14.267	39.520	1.00	84.38	C
ATOM	2579	O	THR	A	334	40.681	14.863	39.898	1.00	85.39	O
ATOM	2580	N	ASP	A	335	42.015	13.048	39.942	1.00	86.59	N
ATOM	2581	CA	ASP	A	335	41.170	12.323	40.883	1.00	86.82	C
ATOM	2582	CB	ASP	A	335	41.831	10.987	41.259	1.00	86.15	C
ATOM	2583	CG	ASP	A	335	40.866	10.010	41.932	1.00	85.99	C
ATOM	2584	OD1	ASP	A	335	41.248	8.832	42.113	1.00	83.51	O
ATOM	2585	OD2	ASP	A	335	39.734	10.414	42.280	1.00	85.66	O
ATOM	2586	C	ASP	A	335	40.973	13.181	42.124	1.00	88.15	C
ATOM	2587	O	ASP	A	335	41.936	13.709	42.681	1.00	87.20	O
ATOM	2588	N	PRO	A	336	39.712	13.365	42.552	1.00	89.83	N
ATOM	2589	CD	PRO	A	336	38.462	12.983	41.873	1.00	88.78	C
ATOM	2590	CA	PRO	A	336	39.432	14.171	43.743	1.00	92.09	C
ATOM	2591	CB	PRO	A	336	37.918	14.373	43.666	1.00	89.50	C
ATOM	2592	CG	PRO	A	336	37.449	13.137	42.969	1.00	88.16	C
ATOM	2593	C	PRO	A	336	39.888	13.449	45.023	1.00	95.49	C
ATOM	2594	O	PRO	A	336	39.595	13.879	46.147	1.00	96.47	O
ATOM	2595	N	GLY	A	337	40.622	12.353	44.833	1.00	97.06	N
ATOM	2596	CA	GLY	A	337	41.128	11.570	45.947	1.00	97.70	C
ATOM	2597	C	GLY	A	337	40.004	10.964	46.759	1.00	97.84	C
ATOM	2598	O	GLY	A	337	38.934	10.659	46.224	1.00	97.55	O
ATOM	2599	N	ASN	A	338	40.253	10.767	48.050	1.00	97.48	N
ATOM	2600	CA	ASN	A	338	39.229	10.229	48.930	1.00	97.08	C
ATOM	2601	CB	ASN	A	338	39.810	9.957	50.319	1.00	97.91	C
ATOM	2602	CG	ASN	A	338	40.612	8.671	50.375	1.00	96.21	C
ATOM	2603	OD1	ASN	A	338	40.059	7.575	50.283	1.00	94.62	O
ATOM	2604	ND2	ASN	A	338	41.924	8.800	50.523	1.00	96.38	N
ATOM	2605	C	ASN	A	338	38.158	11.314	48.987	1.00	97.21	C
ATOM	2606	O	ASN	A	338	38.456	12.485	48.725	1.00	98.02	O
ATOM	2607	N	VAL	A	339	36.926	10.931	49.326	1.00	95.37	N
ATOM	2608	CA	VAL	A	339	35.801	11.872	49.368	1.00	94.13	C
ATOM	2609	CB	VAL	A	339	36.206	13.258	49.961	1.00	95.33	C
ATOM	2610	CG1	VAL	A	339	35.158	14.308	49.616	1.00	95.11	C
ATOM	2611	CG2	VAL	A	339	36.346	13.160	51.467	1.00	95.85	C
ATOM	2612	C	VAL	A	339	35.343	12.071	47.924	1.00	91.62	C
ATOM	2613	O	VAL	A	339	35.824	12.977	47.234	1.00	91.24	O
ATOM	2614	N	GLN	A	340	34.433	11.205	47.477	1.00	86.90	N
ATOM	2615	CA	GLN	A	340	33.904	11.246	46.119	1.00	82.08	C
ATOM	2616	CB	GLN	A	340	33.945	12.683	45.580	1.00	85.23	C
ATOM	2617	CG	GLN	A	340	33.472	12.864	44.153	1.00	90.25	C
ATOM	2618	CD	GLN	A	340	33.659	14.290	43.657	1.00	94.44	C
ATOM	2619	OE1	GLN	A	340	34.770	14.826	43.682	1.00	96.19	O
ATOM	2620	NE2	GLN	A	340	32.571	14.910	43.200	1.00	96.48	N
ATOM	2621	C	GLN	A	340	34.723	10.315	45.226	1.00	76.82	C
ATOM	2622	O	GLN	A	340	35.915	10.537	45.009	1.00	74.65	O
ATOM	2623	N	LYS	A	341	34.073	9.268	44.725	1.00	71.52	N
ATOM	2624	CA	LYS	A	341	34.718	8.290	43.854	1.00	68.10	C
ATOM	2625	CB	LYS	A	341	34.606	6.887	44.461	1.00	69.62	C
ATOM	2626	CG	LYS	A	341	33.201	6.463	44.832	1.00	72.23	C
ATOM	2627	CD	LYS	A	341	32.640	7.283	45.996	1.00	78.15	C
ATOM	2628	CE	LYS	A	341	33.453	7.098	47.281	1.00	78.37	C
ATOM	2629	NZ	LYS	A	341	32.721	7.610	48.480	1.00	72.97	N
ATOM	2630	C	LYS	A	341	34.119	8.306	42.449	1.00	64.62	C

337/396

Figure 3B-48

ATOM	2631	O	LYS	A	341	32.953	7.971	42.261	1.00	63.23	O
ATOM	2632	N	ALA	A	342	34.939	8.675	41.465	1.00	62.41	N
ATOM	2633	CA	ALA	A	342	34.506	8.783	40.070	1.00	61.63	C
ATOM	2634	CB	ALA	A	342	34.704	10.209	39.603	1.00	63.63	C
ATOM	2635	C	ALA	A	342	35.239	7.854	39.129	1.00	59.35	C
ATOM	2636	O	ALA	A	342	36.401	7.574	39.353	1.00	61.58	O
ATOM	2637	N	VAL	A	343	34.586	7.388	38.065	1.00	59.32	N
ATOM	2638	CA	VAL	A	343	35.290	6.506	37.132	1.00	60.29	C
ATOM	2639	CB	VAL	A	343	34.386	6.002	35.920	1.00	55.47	C
ATOM	2640	CG1	VAL	A	343	32.950	5.848	36.360	1.00	49.54	C
ATOM	2641	CG2	VAL	A	343	34.518	6.911	34.710	1.00	55.98	C
ATOM	2642	C	VAL	A	343	36.475	7.345	36.634	1.00	62.42	C
ATOM	2643	O	VAL	A	343	36.293	8.442	36.094	1.00	61.19	O
ATOM	2644	N	CYS	A	344	37.690	6.838	36.849	1.00	63.76	N
ATOM	2645	CA	CYS	A	344	38.889	7.576	36.464	1.00	63.90	C
ATOM	2646	C	CYS	A	344	39.333	7.469	35.018	1.00	60.99	C
ATOM	2647	O	CYS	A	344	40.208	8.231	34.576	1.00	58.06	O
ATOM	2648	CB	CYS	A	344	40.056	7.200	37.377	1.00	66.59	C
ATOM	2649	SG	CYS	A	344	40.296	8.303	38.816	1.00	72.59	S
ATOM	2650	N	HIS	A	345	38.735	6.528	34.291	1.00	58.06	N
ATOM	2651	CA	HIS	A	345	39.069	6.331	32.891	1.00	54.90	C
ATOM	2652	CB	HIS	A	345	38.136	5.302	32.267	1.00	52.86	C
ATOM	2653	CG	HIS	A	345	38.694	4.667	31.036	1.00	56.18	C
ATOM	2654	CD2	HIS	A	345	38.713	5.084	29.749	1.00	58.08	C
ATOM	2655	ND1	HIS	A	345	39.396	3.480	31.062	1.00	58.02	N
ATOM	2656	CE1	HIS	A	345	39.823	3.197	29.846	1.00	58.34	C
ATOM	2657	NE2	HIS	A	345	39.422	4.155	29.029	1.00	55.50	N
ATOM	2658	C	HIS	A	345	38.893	7.679	32.205	1.00	54.55	C
ATOM	2659	O	HIS	A	345	37.840	8.311	32.322	1.00	59.55	O
ATOM	2660	N	PRO	A	346	39.924	8.150	31.492	1.00	51.76	N
ATOM	2661	CD	PRO	A	346	41.184	7.464	31.187	1.00	51.05	C
ATOM	2662	CA	PRO	A	346	39.856	9.440	30.796	1.00	50.81	C
ATOM	2663	CB	PRO	A	346	41.248	9.590	30.167	1.00	52.00	C
ATOM	2664	CG	PRO	A	346	42.106	8.624	30.902	1.00	49.73	C
ATOM	2665	C	PRO	A	346	38.776	9.420	29.725	1.00	49.78	C
ATOM	2666	O	PRO	A	346	38.763	8.553	28.850	1.00	49.71	O
ATOM	2667	N	THR	A	347	37.869	10.374	29.779	1.00	47.59	N
ATOM	2668	CA	THR	A	347	36.829	10.403	28.777	1.00	47.32	C
ATOM	2669	CB	THR	A	347	35.561	9.742	29.315	1.00	45.18	C
ATOM	2670	OG1	THR	A	347	34.953	10.587	30.295	1.00	43.50	O
ATOM	2671	CG2	THR	A	347	35.907	8.411	29.956	1.00	40.75	C
ATOM	2672	C	THR	A	347	36.551	11.838	28.384	1.00	48.14	C
ATOM	2673	O	THR	A	347	36.650	12.723	29.224	1.00	51.52	O
ATOM	2674	N	ALA	A	348	36.242	12.079	27.109	1.00	49.06	N
ATOM	2675	CA	ALA	A	348	35.942	13.437	26.636	1.00	50.29	C
ATOM	2676	CB	ALA	A	348	36.597	13.684	25.310	1.00	51.22	C
ATOM	2677	C	ALA	A	348	34.447	13.556	26.491	1.00	49.40	C
ATOM	2678	O	ALA	A	348	33.878	12.959	25.603	1.00	53.18	O
ATOM	2679	N	TRP	A	349	33.809	14.327	27.355	1.00	51.48	N
ATOM	2680	CA	TRP	A	349	32.360	14.461	27.308	1.00	54.43	C
ATOM	2681	CB	TRP	A	349	31.811	14.746	28.710	1.00	49.62	C
ATOM	2682	CG	TRP	A	349	31.877	13.567	29.640	1.00	47.33	C
ATOM	2683	CD2	TRP	A	349	30.786	12.987	30.365	1.00	44.44	C
ATOM	2684	CE2	TRP	A	349	31.301	11.878	31.077	1.00	43.58	C
ATOM	2685	CE3	TRP	A	349	29.421	13.286	30.471	1.00	42.95	C
ATOM	2686	CD1	TRP	A	349	32.981	12.815	29.945	1.00	43.77	C

338/396

Figure 3B-49

ATOM	2687	NE1	TRP	A	349	32.642	11.802	30.804	1.00	39.79	N
ATOM	2688	CZ2	TRP	A	349	30.499	11.073	31.899	1.00	45.64	C
ATOM	2689	CZ3	TRP	A	349	28.624	12.485	31.287	1.00	46.01	C
ATOM	2690	CH2	TRP	A	349	29.168	11.385	31.987	1.00	44.85	C
ATOM	2691	C	TRP	A	349	31.834	15.517	26.353	1.00	58.80	C
ATOM	2692	O	TRP	A	349	32.501	16.506	26.057	1.00	60.64	O
ATOM	2693	N	ASP	A	350	30.625	15.274	25.862	1.00	63.07	N
ATOM	2694	CA	ASP	A	350	29.928	16.194	24.972	1.00	64.73	C
ATOM	2695	CB	ASP	A	350	29.977	15.706	23.516	1.00	71.09	C
ATOM	2696	CG	ASP	A	350	29.329	16.696	22.537	1.00	76.57	C
ATOM	2697	OD1	ASP	A	350	29.440	16.500	21.302	1.00	77.21	O
ATOM	2698	OD2	ASP	A	350	28.705	17.671	23.009	1.00	79.32	O
ATOM	2699	C	ASP	A	350	28.498	16.179	25.494	1.00	62.94	C
ATOM	2700	O	ASP	A	350	27.710	15.307	25.153	1.00	63.51	O
ATOM	2701	N	LEU	A	351	28.171	17.119	26.366	1.00	60.96	N
ATOM	2702	CA	LEU	A	351	26.828	17.152	26.906	1.00	63.15	C
ATOM	2703	CB	LEU	A	351	26.841	17.778	28.304	1.00	58.57	C
ATOM	2704	CG	LEU	A	351	27.854	17.275	29.324	1.00	49.75	C
ATOM	2705	CD1	LEU	A	351	29.113	18.073	29.207	1.00	49.28	C
ATOM	2706	CD2	LEU	A	351	27.305	17.448	30.701	1.00	51.05	C
ATOM	2707	C	LEU	A	351	25.951	17.970	25.947	1.00	67.01	C
ATOM	2708	O	LEU	A	351	24.747	18.170	26.173	1.00	66.48	O
ATOM	2709	N	GLY	A	352	26.576	18.433	24.867	1.00	68.80	N
ATOM	2710	CA	GLY	A	352	25.871	19.218	23.875	1.00	70.55	C
ATOM	2711	C	GLY	A	352	25.430	20.539	24.454	1.00	72.74	C
ATOM	2712	O	GLY	A	352	25.810	20.884	25.573	1.00	75.26	O
ATOM	2713	N	LYS	A	353	24.624	21.277	23.699	1.00	72.21	N
ATOM	2714	CA	LYS	A	353	24.137	22.571	24.153	1.00	71.44	C
ATOM	2715	CB	LYS	A	353	23.311	22.401	25.433	1.00	71.55	C
ATOM	2716	CG	LYS	A	353	22.636	23.659	25.935	1.00	77.22	C
ATOM	2717	CD	LYS	A	353	21.753	24.334	24.862	1.00	86.44	C
ATOM	2718	CE	LYS	A	353	22.540	25.321	23.962	1.00	88.39	C
ATOM	2719	NZ	LYS	A	353	21.708	26.019	22.920	1.00	88.33	N
ATOM	2720	C	LYS	A	353	25.329	23.495	24.390	1.00	70.93	C
ATOM	2721	O	LYS	A	353	25.227	24.498	25.095	1.00	70.81	O
ATOM	2722	N	GLY	A	354	26.464	23.140	23.789	1.00	70.13	N
ATOM	2723	CA	GLY	A	354	27.666	23.943	23.923	1.00	68.18	C
ATOM	2724	C	GLY	A	354	28.532	23.584	25.110	1.00	68.20	C
ATOM	2725	O	GLY	A	354	29.542	24.234	25.364	1.00	65.53	O
ATOM	2726	N	ASP	A	355	28.153	22.531	25.825	1.00	70.34	N
ATOM	2727	CA	ASP	A	355	28.898	22.102	27.006	1.00	73.15	C
ATOM	2728	CB	ASP	A	355	27.916	21.631	28.076	1.00	72.08	C
ATOM	2729	CG	ASP	A	355	28.594	21.351	29.386	1.00	72.42	C
ATOM	2730	OD1	ASP	A	355	27.911	20.840	30.297	1.00	71.65	O
ATOM	2731	OD2	ASP	A	355	29.809	21.648	29.496	1.00	70.70	O
ATOM	2732	C	ASP	A	355	29.952	21.008	26.762	1.00	74.24	C
ATOM	2733	O	ASP	A	355	29.622	19.848	26.510	1.00	73.83	O
ATOM	2734	N	PHE	A	356	31.222	21.385	26.867	1.00	76.07	N
ATOM	2735	CA	PHE	A	356	32.319	20.445	26.646	1.00	78.34	C
ATOM	2736	CB	PHE	A	356	33.221	20.950	25.512	1.00	79.84	C
ATOM	2737	CG	PHE	A	356	32.494	21.203	24.219	1.00	82.19	C
ATOM	2738	CD1	PHE	A	356	31.540	22.196	24.127	1.00	82.81	C
ATOM	2739	CD2	PHE	A	356	32.768	20.445	23.095	1.00	84.64	C
ATOM	2740	CE1	PHE	A	356	30.876	22.427	22.939	1.00	83.26	C
ATOM	2741	CE2	PHE	A	356	32.103	20.676	21.907	1.00	84.84	C
ATOM	2742	CZ	PHE	A	356	31.159	21.666	21.831	1.00	82.54	C

339/396

Figure 3B-50

ATOM	2743	C	PHE	A	356	33.160	20.220	27.909	1.00	77.92	C
ATOM	2744	O	PHE	A	356	33.590	21.172	28.567	1.00	78.63	O
ATOM	2745	N	ARG	A	357	33.398	18.955	28.238	1.00	75.02	N
ATOM	2746	CA	ARG	A	357	34.174	18.613	29.423	1.00	71.84	C
ATOM	2747	CB	ARG	A	357	33.231	18.364	30.606	1.00	70.17	C
ATOM	2748	CG	ARG	A	357	32.245	19.483	30.901	1.00	70.94	C
ATOM	2749	CD	ARG	A	357	31.349	19.114	32.093	1.00	74.61	C
ATOM	2750	NE	ARG	A	357	30.331	20.121	32.411	1.00	73.55	N
ATOM	2751	CZ	ARG	A	357	29.431	19.995	33.385	1.00	73.17	C
ATOM	2752	NH1	ARG	A	357	28.541	20.951	33.601	1.00	72.08	N
ATOM	2753	NH2	ARG	A	357	29.418	18.913	34.149	1.00	73.90	N
ATOM	2754	C	ARG	A	357	35.043	17.367	29.206	1.00	69.27	C
ATOM	2755	O	ARG	A	357	34.867	16.627	28.240	1.00	70.87	O
ATOM	2756	N	ILE	A	358	35.984	17.145	30.116	1.00	64.08	N
ATOM	2757	CA	ILE	A	358	36.853	15.979	30.053	1.00	58.31	C
ATOM	2758	CB	ILE	A	358	38.201	16.285	29.424	1.00	53.48	C
ATOM	2759	CG2	ILE	A	358	39.222	15.268	29.914	1.00	50.21	C
ATOM	2760	CG1	ILE	A	358	38.079	16.290	27.906	1.00	48.36	C
ATOM	2761	CD1	ILE	A	358	39.369	16.588	27.204	1.00	44.36	C
ATOM	2762	C	ILE	A	358	37.138	15.482	31.450	1.00	58.32	C
ATOM	2763	O	ILE	A	358	37.782	16.169	32.229	1.00	60.98	O
ATOM	2764	N	LEU	A	359	36.659	14.289	31.767	1.00	55.77	N
ATOM	2765	CA	LEU	A	359	36.884	13.706	33.077	1.00	53.08	C
ATOM	2766	CB	LEU	A	359	35.626	12.959	33.510	1.00	46.26	C
ATOM	2767	CG	LEU	A	359	35.637	12.142	34.792	1.00	45.49	C
ATOM	2768	CD1	LEU	A	359	34.223	11.929	35.264	1.00	42.25	C
ATOM	2769	CD2	LEU	A	359	36.318	10.811	34.545	1.00	49.11	C
ATOM	2770	C	LEU	A	359	38.097	12.774	33.006	1.00	54.33	C
ATOM	2771	O	LEU	A	359	38.019	11.683	32.444	1.00	54.13	O
ATOM	2772	N	MET	A	360	39.222	13.214	33.565	1.00	55.85	N
ATOM	2773	CA	MET	A	360	40.451	12.419	33.548	1.00	60.98	C
ATOM	2774	CB	MET	A	360	41.297	12.795	32.322	1.00	61.82	C
ATOM	2775	CG	MET	A	360	42.611	12.032	32.190	1.00	60.14	C
ATOM	2776	SD	MET	A	360	43.550	12.537	30.738	1.00	64.60	S
ATOM	2777	CE	MET	A	360	45.168	11.830	31.069	1.00	58.48	C
ATOM	2778	C	MET	A	360	41.299	12.594	34.810	1.00	62.61	C
ATOM	2779	O	MET	A	360	41.631	13.715	35.181	1.00	62.45	O
ATOM	2780	N	CYS	A	361	41.649	11.489	35.469	1.00	63.31	N
ATOM	2781	CA	CYS	A	361	42.476	11.568	36.669	1.00	62.79	C
ATOM	2782	C	CYS	A	361	43.918	11.644	36.190	1.00	62.78	C
ATOM	2783	O	CYS	A	361	44.676	10.677	36.268	1.00	62.98	O
ATOM	2784	CB	CYS	A	361	42.246	10.344	37.560	1.00	62.16	C
ATOM	2785	SG	CYS	A	361	40.490	10.171	38.020	1.00	68.02	S
ATOM	2786	N	THR	A	362	44.283	12.818	35.685	1.00	63.11	N
ATOM	2787	CA	THR	A	362	45.617	13.056	35.145	1.00	62.76	C
ATOM	2788	CB	THR	A	362	45.756	14.475	34.573	1.00	58.29	C
ATOM	2789	OG1	THR	A	362	44.523	14.867	33.966	1.00	59.12	O
ATOM	2790	CG2	THR	A	362	46.840	14.508	33.518	1.00	53.19	C
ATOM	2791	C	THR	A	362	46.752	12.855	36.128	1.00	65.06	C
ATOM	2792	O	THR	A	362	46.701	13.292	37.277	1.00	69.21	O
ATOM	2793	N	LYS	A	363	47.787	12.186	35.653	1.00	65.44	N
ATOM	2794	CA	LYS	A	363	48.965	11.929	36.448	1.00	65.67	C
ATOM	2795	CB	LYS	A	363	49.135	10.413	36.612	1.00	65.70	C
ATOM	2796	CG	LYS	A	363	47.941	9.783	37.344	1.00	69.59	C
ATOM	2797	CD	LYS	A	363	47.425	8.472	36.729	1.00	72.67	C
ATOM	2798	CE	LYS	A	363	48.285	7.261	37.099	1.00	73.59	C

340/396

Figure 3B-51

ATOM	2799	NZ	LYS	A	363	47.671	5.969	36.659	1.00	68.79	N
ATOM	2800	C	LYS	A	363	50.070	12.569	35.609	1.00	65.71	C
ATOM	2801	O	LYS	A	363	49.885	12.779	34.409	1.00	65.79	O
ATOM	2802	N	VAL	A	364	51.195	12.914	36.229	1.00	64.36	N
ATOM	2803	CA	VAL	A	364	52.287	13.542	35.501	1.00	63.28	C
ATOM	2804	CB	VAL	A	364	53.118	14.421	36.426	1.00	60.70	C
ATOM	2805	CG1	VAL	A	364	54.107	15.218	35.614	1.00	63.44	C
ATOM	2806	CG2	VAL	A	364	52.218	15.341	37.202	1.00	56.84	C
ATOM	2807	C	VAL	A	364	53.199	12.511	34.849	1.00	64.88	C
ATOM	2808	O	VAL	A	364	54.351	12.370	35.230	1.00	65.52	O
ATOM	2809	N	THR	A	365	52.664	11.804	33.858	1.00	66.62	N
ATOM	2810	CA	THR	A	365	53.375	10.765	33.116	1.00	67.53	C
ATOM	2811	CB	THR	A	365	52.594	9.436	33.180	1.00	68.58	C
ATOM	2812	OG1	THR	A	365	52.319	9.110	34.546	1.00	69.69	O
ATOM	2813	CG2	THR	A	365	53.381	8.312	32.539	1.00	70.49	C
ATOM	2814	C	THR	A	365	53.392	11.228	31.664	1.00	68.77	C
ATOM	2815	O	THR	A	365	52.635	12.130	31.313	1.00	69.92	O
ATOM	2816	N	MET	A	366	54.239	10.639	30.819	1.00	69.74	N
ATOM	2817	CA	MET	A	366	54.242	11.035	29.404	1.00	70.86	C
ATOM	2818	CB	MET	A	366	55.512	10.577	28.681	1.00	68.91	C
ATOM	2819	CG	MET	A	366	55.665	11.174	27.276	1.00	65.53	C
ATOM	2820	SD	MET	A	366	57.034	10.463	26.314	1.00	64.30	S
ATOM	2821	CE	MET	A	366	57.062	11.531	24.887	1.00	61.17	C
ATOM	2822	C	MET	A	366	53.027	10.362	28.767	1.00	71.44	C
ATOM	2823	O	MET	A	366	52.587	10.730	27.679	1.00	70.90	O
ATOM	2824	N	ASP	A	367	52.505	9.359	29.465	1.00	71.47	N
ATOM	2825	CA	ASP	A	367	51.337	8.638	29.018	1.00	69.90	C
ATOM	2826	CB	ASP	A	367	51.080	7.430	29.913	1.00	72.57	C
ATOM	2827	CG	ASP	A	367	51.215	6.118	29.166	1.00	76.34	C
ATOM	2828	OD1	ASP	A	367	51.199	5.045	29.809	1.00	78.54	O
ATOM	2829	OD2	ASP	A	367	51.332	6.159	27.925	1.00	79.53	O
ATOM	2830	C	ASP	A	367	50.191	9.609	29.133	1.00	70.34	C
ATOM	2831	O	ASP	A	367	49.428	9.779	28.195	1.00	73.66	O
ATOM	2832	N	ASP	A	368	50.076	10.259	30.286	1.00	70.27	N
ATOM	2833	CA	ASP	A	368	49.002	11.222	30.495	1.00	70.46	C
ATOM	2834	CB	ASP	A	368	48.792	11.491	31.989	1.00	72.35	C
ATOM	2835	CG	ASP	A	368	48.259	10.277	32.729	1.00	74.57	C
ATOM	2836	OD1	ASP	A	368	48.939	9.230	32.694	1.00	80.37	O
ATOM	2837	OD2	ASP	A	368	47.165	10.357	33.338	1.00	70.97	O
ATOM	2838	C	ASP	A	368	49.285	12.523	29.756	1.00	69.19	C
ATOM	2839	O	ASP	A	368	48.484	13.446	29.784	1.00	69.98	O
ATOM	2840	N	PHE	A	369	50.433	12.600	29.099	1.00	68.23	N
ATOM	2841	CA	PHE	A	369	50.765	13.788	28.320	1.00	68.73	C
ATOM	2842	CB	PHE	A	369	52.272	13.886	28.105	1.00	68.43	C
ATOM	2843	CG	PHE	A	369	52.673	14.878	27.044	1.00	69.34	C
ATOM	2844	CD1	PHE	A	369	53.200	14.443	25.834	1.00	70.52	C
ATOM	2845	CD2	PHE	A	369	52.559	16.243	27.267	1.00	65.17	C
ATOM	2846	CE1	PHE	A	369	53.613	15.350	24.871	1.00	68.00	C
ATOM	2847	CE2	PHE	A	369	52.966	17.149	26.312	1.00	62.46	C
ATOM	2848	CZ	PHE	A	369	53.496	16.704	25.113	1.00	65.89	C
ATOM	2849	C	PHE	A	369	50.072	13.649	26.969	1.00	68.98	C
ATOM	2850	O	PHE	A	369	49.508	14.606	26.439	1.00	69.66	O
ATOM	2851	N	LEU	A	370	50.124	12.433	26.430	1.00	67.88	N
ATOM	2852	CA	LEU	A	370	49.510	12.099	25.157	1.00	65.65	C
ATOM	2853	CB	LEU	A	370	50.187	10.872	24.561	1.00	65.91	C
ATOM	2854	CG	LEU	A	370	51.696	11.057	24.435	1.00	67.45	C

341/396

Figure 3B-52

ATOM	2855	CD1	LEU	A	370	52.279	9.984	23.520	1.00	64.61	C
ATOM	2856	CD2	LEU	A	370	51.973	12.445	23.874	1.00	68.95	C
ATOM	2857	C	LEU	A	370	48.007	11.851	25.266	1.00	64.53	C
ATOM	2858	O	LEU	A	370	47.246	12.403	24.481	1.00	65.24	O
ATOM	2859	N	THR	A	371	47.573	11.031	26.224	1.00	62.33	N
ATOM	2860	CA	THR	A	371	46.140	10.760	26.375	1.00	61.71	C
ATOM	2861	CB	THR	A	371	45.822	9.972	27.653	1.00	58.14	C
ATOM	2862	OG1	THR	A	371	46.322	8.640	27.532	1.00	56.18	O
ATOM	2863	CG2	THR	A	371	44.320	9.910	27.870	1.00	56.05	C
ATOM	2864	C	THR	A	371	45.346	12.060	26.413	1.00	64.44	C
ATOM	2865	O	THR	A	371	44.165	12.102	26.037	1.00	65.62	O
ATOM	2866	N	ALA	A	372	46.001	13.121	26.877	1.00	63.83	N
ATOM	2867	CA	ALA	A	372	45.379	14.429	26.942	1.00	59.44	C
ATOM	2868	CB	ALA	A	372	46.241	15.359	27.746	1.00	62.21	C
ATOM	2869	C	ALA	A	372	45.237	14.925	25.499	1.00	56.57	C
ATOM	2870	O	ALA	A	372	44.205	15.483	25.133	1.00	55.77	O
ATOM	2871	N	HIS	A	373	46.273	14.720	24.685	1.00	50.58	N
ATOM	2872	CA	HIS	A	373	46.216	15.110	23.277	1.00	49.20	C
ATOM	2873	CB	HIS	A	373	47.533	14.847	22.564	1.00	48.25	C
ATOM	2874	CG	HIS	A	373	48.532	15.941	22.718	1.00	50.80	C
ATOM	2875	CD2	HIS	A	373	49.289	16.587	21.802	1.00	53.01	C
ATOM	2876	ND1	HIS	A	373	48.900	16.443	23.945	1.00	53.90	N
ATOM	2877	CE1	HIS	A	373	49.846	17.351	23.780	1.00	54.76	C
ATOM	2878	NE2	HIS	A	373	50.101	17.456	22.489	1.00	54.98	N
ATOM	2879	C	HIS	A	373	45.161	14.253	22.612	1.00	48.03	C
ATOM	2880	O	HIS	A	373	44.620	14.601	21.570	1.00	51.41	O
ATOM	2881	N	HIS	A	374	44.894	13.099	23.195	1.00	44.25	N
ATOM	2882	CA	HIS	A	374	43.890	12.252	22.629	1.00	40.08	C
ATOM	2883	CB	HIS	A	374	43.898	10.887	23.259	1.00	35.35	C
ATOM	2884	CG	HIS	A	374	42.878	9.966	22.679	1.00	34.42	C
ATOM	2885	CD2	HIS	A	374	41.644	9.613	23.108	1.00	30.22	C
ATOM	2886	ND1	HIS	A	374	43.071	9.303	21.486	1.00	35.20	N
ATOM	2887	CE1	HIS	A	374	42.003	8.577	21.211	1.00	33.10	C
ATOM	2888	NE2	HIS	A	374	41.122	8.749	22.178	1.00	31.90	N
ATOM	2889	C	HIS	A	374	42.617	12.927	23.019	1.00	43.89	C
ATOM	2890	O	HIS	A	374	42.031	13.671	22.242	1.00	46.85	O
ATOM	2891	N	GLU	A	375	42.206	12.673	24.254	1.00	45.89	N
ATOM	2892	CA	GLU	A	375	40.974	13.234	24.790	1.00	47.33	C
ATOM	2893	CB	GLU	A	375	41.046	13.263	26.318	1.00	48.98	C
ATOM	2894	CG	GLU	A	375	41.246	11.877	26.916	1.00	51.88	C
ATOM	2895	CD	GLU	A	375	40.256	10.860	26.363	1.00	53.02	C
ATOM	2896	OE1	GLU	A	375	39.040	11.032	26.567	1.00	55.79	O
ATOM	2897	OE2	GLU	A	375	40.689	9.891	25.718	1.00	51.48	O
ATOM	2898	C	GLU	A	375	40.641	14.614	24.238	1.00	45.98	C
ATOM	2899	O	GLU	A	375	39.511	14.869	23.862	1.00	41.45	O
ATOM	2900	N	MET	A	376	41.623	15.503	24.179	1.00	49.64	N
ATOM	2901	CA	MET	A	376	41.368	16.838	23.653	1.00	52.72	C
ATOM	2902	CB	MET	A	376	42.630	17.709	23.741	1.00	54.33	C
ATOM	2903	CG	MET	A	376	42.342	19.209	23.639	1.00	57.59	C
ATOM	2904	SD	MET	A	376	43.447	20.317	24.591	1.00	62.44	S
ATOM	2905	CE	MET	A	376	42.694	20.186	26.211	1.00	54.88	C
ATOM	2906	C	MET	A	376	40.877	16.715	22.203	1.00	52.70	C
ATOM	2907	O	MET	A	376	39.812	17.229	21.869	1.00	54.84	O
ATOM	2908	N	GLY	A	377	41.638	16.030	21.350	1.00	49.12	N
ATOM	2909	CA	GLY	A	377	41.210	15.845	19.975	1.00	46.15	C
ATOM	2910	C	GLY	A	377	39.752	15.408	19.927	1.00	45.52	C

342/396

Figure 3B-53

ATOM	2911	O	GLY	A	377	38.957	15.868	19.123	1.00	45.01	O
ATOM	2912	N	HIS	A	378	39.383	14.501	20.807	1.00	47.33	N
ATOM	2913	CA	HIS	A	378	38.008	14.048	20.842	1.00	48.77	C
ATOM	2914	CB	HIS	A	378	37.783	13.182	22.080	1.00	45.64	C
ATOM	2915	CG	HIS	A	378	37.445	11.768	21.761	1.00	46.25	C
ATOM	2916	CD2	HIS	A	378	36.584	10.901	22.342	1.00	51.45	C
ATOM	2917	ND1	HIS	A	378	38.011	11.095	20.702	1.00	46.49	N
ATOM	2918	CE1	HIS	A	378	37.508	9.876	20.639	1.00	48.41	C
ATOM	2919	NE2	HIS	A	378	36.639	9.732	21.623	1.00	49.31	N
ATOM	2920	C	HIS	A	378	37.124	15.277	20.899	1.00	49.97	C
ATOM	2921	O	HIS	A	378	36.094	15.348	20.254	1.00	53.80	O
ATOM	2922	N	ILE	A	379	37.552	16.258	21.674	1.00	51.00	N
ATOM	2923	CA	ILE	A	379	36.798	17.480	21.842	1.00	51.42	C
ATOM	2924	CB	ILE	A	379	37.335	18.280	23.013	1.00	47.66	C
ATOM	2925	CG2	ILE	A	379	36.747	19.664	22.996	1.00	49.92	C
ATOM	2926	CG1	ILE	A	379	37.024	17.550	24.308	1.00	44.75	C
ATOM	2927	CD1	ILE	A	379	35.585	17.205	24.458	1.00	44.74	C
ATOM	2928	C	ILE	A	379	36.828	18.365	20.615	1.00	55.34	C
ATOM	2929	O	ILE	A	379	35.783	18.745	20.091	1.00	57.98	O
ATOM	2930	N	GLN	A	380	38.031	18.701	20.163	1.00	57.49	N
ATOM	2931	CA	GLN	A	380	38.191	19.562	19.001	1.00	56.87	C
ATOM	2932	CB	GLN	A	380	39.637	19.552	18.517	1.00	57.05	C
ATOM	2933	CG	GLN	A	380	40.100	20.894	17.996	1.00	60.60	C
ATOM	2934	CD	GLN	A	380	40.266	21.909	19.109	1.00	62.16	C
ATOM	2935	OE1	GLN	A	380	41.351	22.456	19.310	1.00	63.25	O
ATOM	2936	NE2	GLN	A	380	39.190	22.161	19.844	1.00	62.94	N
ATOM	2937	C	GLN	A	380	37.276	19.085	17.896	1.00	55.60	C
ATOM	2938	O	GLN	A	380	36.853	19.868	17.062	1.00	57.10	O
ATOM	2939	N	TYR	A	381	36.976	17.793	17.908	1.00	54.86	N
ATOM	2940	CA	TYR	A	381	36.099	17.182	16.924	1.00	54.97	C
ATOM	2941	CB	TYR	A	381	36.334	15.671	16.901	1.00	57.49	C
ATOM	2942	CG	TYR	A	381	35.900	14.946	15.642	1.00	59.80	C
ATOM	2943	CD1	TYR	A	381	35.784	13.568	15.626	1.00	60.79	C
ATOM	2944	CE1	TYR	A	381	35.415	12.897	14.484	1.00	62.44	C
ATOM	2945	CD2	TYR	A	381	35.629	15.630	14.470	1.00	62.79	C
ATOM	2946	CE2	TYR	A	381	35.256	14.959	13.315	1.00	61.32	C
ATOM	2947	CZ	TYR	A	381	35.152	13.593	13.330	1.00	61.17	C
ATOM	2948	OH	TYR	A	381	34.798	12.908	12.188	1.00	61.83	O
ATOM	2949	C	TYR	A	381	34.662	17.495	17.349	1.00	55.07	C
ATOM	2950	O	TYR	A	381	33.943	18.190	16.640	1.00	54.89	O
ATOM	2951	N	ASP	A	382	34.250	16.989	18.509	1.00	55.91	N
ATOM	2952	CA	ASP	A	382	32.902	17.240	19.027	1.00	57.50	C
ATOM	2953	CB	ASP	A	382	32.848	16.995	20.546	1.00	60.23	C
ATOM	2954	CG	ASP	A	382	33.040	15.530	20.932	1.00	61.26	C
ATOM	2955	OD1	ASP	A	382	32.248	14.677	20.474	1.00	62.29	O
ATOM	2956	OD2	ASP	A	382	33.974	15.237	21.712	1.00	59.22	O
ATOM	2957	C	ASP	A	382	32.453	18.684	18.743	1.00	58.24	C
ATOM	2958	O	ASP	A	382	31.264	18.948	18.549	1.00	55.05	O
ATOM	2959	N	MET	A	383	33.413	19.612	18.747	1.00	60.39	N
ATOM	2960	CA	MET	A	383	33.153	21.028	18.481	1.00	61.32	C
ATOM	2961	CB	MET	A	383	34.315	21.899	18.945	1.00	59.06	C
ATOM	2962	CG	MET	A	383	34.699	21.760	20.402	1.00	62.33	C
ATOM	2963	SD	MET	A	383	35.724	23.158	20.939	1.00	57.87	S
ATOM	2964	CE	MET	A	383	34.406	24.264	21.402	1.00	60.73	C
ATOM	2965	C	MET	A	383	33.001	21.233	16.984	1.00	63.56	C
ATOM	2966	O	MET	A	383	31.954	21.642	16.496	1.00	63.77	O

343/396

Figure 3B-54

ATOM	2967	N	ALA	A	384	34.078	20.946	16.265	1.00	65.23	N
ATOM	2968	CA	ALA	A	384	34.111	21.083	14.819	1.00	64.96	C
ATOM	2969	CB	ALA	A	384	35.302	20.342	14.252	1.00	61.69	C
ATOM	2970	C	ALA	A	384	32.841	20.598	14.142	1.00	66.45	C
ATOM	2971	O	ALA	A	384	32.527	21.046	13.046	1.00	72.88	O
ATOM	2972	N	TYR	A	385	32.101	19.688	14.760	1.00	64.21	N
ATOM	2973	CA	TYR	A	385	30.888	19.230	14.102	1.00	64.32	C
ATOM	2974	CB	TYR	A	385	30.970	17.713	13.798	1.00	64.83	C
ATOM	2975	CG	TYR	A	385	30.943	16.753	14.986	1.00	61.95	C
ATOM	2976	CD1	TYR	A	385	31.805	15.668	15.049	1.00	58.47	C
ATOM	2977	CE1	TYR	A	385	31.742	14.771	16.089	1.00	57.40	C
ATOM	2978	CD2	TYR	A	385	30.023	16.902	16.005	1.00	62.53	C
ATOM	2979	CE2	TYR	A	385	29.955	16.013	17.040	1.00	61.92	C
ATOM	2980	CZ	TYR	A	385	30.812	14.950	17.081	1.00	59.15	C
ATOM	2981	OH	TYR	A	385	30.707	14.072	18.136	1.00	61.67	O
ATOM	2982	C	TYR	A	385	29.644	19.587	14.900	1.00	65.44	C
ATOM	2983	O	TYR	A	385	28.545	19.090	14.624	1.00	66.08	O
ATOM	2984	N	ALA	A	386	29.825	20.465	15.888	1.00	65.85	N
ATOM	2985	CA	ALA	A	386	28.725	20.916	16.749	1.00	64.90	C
ATOM	2986	CB	ALA	A	386	29.245	21.898	17.799	1.00	64.10	C
ATOM	2987	C	ALA	A	386	27.674	21.586	15.880	1.00	62.76	C
ATOM	2988	O	ALA	A	386	26.491	21.249	15.933	1.00	59.79	O
ATOM	2989	N	ALA	A	387	28.130	22.542	15.082	1.00	61.55	N
ATOM	2990	CA	ALA	A	387	27.264	23.254	14.166	1.00	62.13	C
ATOM	2991	CB	ALA	A	387	28.028	24.412	13.550	1.00	60.47	C
ATOM	2992	C	ALA	A	387	26.873	22.240	13.093	1.00	61.67	C
ATOM	2993	O	ALA	A	387	27.508	22.166	12.046	1.00	66.55	O
ATOM	2994	N	GLN	A	388	25.834	21.459	13.346	1.00	58.03	N
ATOM	2995	CA	GLN	A	388	25.432	20.437	12.389	1.00	58.42	C
ATOM	2996	CB	GLN	A	388	26.613	19.494	12.152	1.00	59.59	C
ATOM	2997	CG	GLN	A	388	26.322	18.303	11.271	1.00	58.11	C
ATOM	2998	CD	GLN	A	388	27.012	18.403	9.935	1.00	56.62	C
ATOM	2999	OE1	GLN	A	388	26.685	17.672	9.010	1.00	61.22	O
ATOM	3000	NE2	GLN	A	388	27.978	19.303	9.831	1.00	49.80	N
ATOM	3001	C	GLN	A	388	24.266	19.655	12.977	1.00	59.51	C
ATOM	3002	O	GLN	A	388	24.240	19.396	14.178	1.00	63.15	O
ATOM	3003	N	PRO	A	389	23.295	19.252	12.143	1.00	56.86	N
ATOM	3004	CD	PRO	A	389	23.406	19.124	10.689	1.00	58.00	C
ATOM	3005	CA	PRO	A	389	22.137	18.498	12.624	1.00	56.78	C
ATOM	3006	CB	PRO	A	389	21.610	17.829	11.358	1.00	55.54	C
ATOM	3007	CG	PRO	A	389	22.807	17.763	10.482	1.00	58.76	C
ATOM	3008	C	PRO	A	389	22.475	17.495	13.716	1.00	59.72	C
ATOM	3009	O	PRO	A	389	23.161	16.505	13.479	1.00	61.30	O
ATOM	3010	N	PHE	A	390	21.983	17.772	14.919	1.00	62.07	N
ATOM	3011	CA	PHE	A	390	22.198	16.938	16.108	1.00	60.92	C
ATOM	3012	CB	PHE	A	390	21.074	17.194	17.105	1.00	56.44	C
ATOM	3013	CG	PHE	A	390	21.028	16.233	18.249	1.00	51.31	C
ATOM	3014	CD1	PHE	A	390	21.540	16.586	19.483	1.00	55.43	C
ATOM	3015	CD2	PHE	A	390	20.380	15.020	18.124	1.00	49.53	C
ATOM	3016	CE1	PHE	A	390	21.392	15.745	20.579	1.00	54.82	C
ATOM	3017	CE2	PHE	A	390	20.231	14.178	19.206	1.00	49.98	C
ATOM	3018	CZ	PHE	A	390	20.732	14.539	20.436	1.00	51.79	C
ATOM	3019	C	PHE	A	390	22.306	15.443	15.866	1.00	61.17	C
ATOM	3020	O	PHE	A	390	23.255	14.812	16.311	1.00	62.45	O
ATOM	3021	N	LEU	A	391	21.329	14.874	15.175	1.00	61.04	N
ATOM	3022	CA	LEU	A	391	21.342	13.444	14.928	1.00	61.17	C

344/396

Figure 3B-55

ATOM	3023	CB	LEU	A	391	19.927	12.960	14.620	1.00	61.09	C
ATOM	3024	CG	LEU	A	391	19.699	11.479	14.900	1.00	60.21	C
ATOM	3025	CD1	LEU	A	391	21.041	10.841	15.255	1.00	62.90	C
ATOM	3026	CD2	LEU	A	391	18.714	11.295	16.041	1.00	57.35	C
ATOM	3027	C	LEU	A	391	22.276	13.103	13.778	1.00	62.77	C
ATOM	3028	O	LEU	A	391	22.004	12.210	12.978	1.00	66.12	O
ATOM	3029	N	LEU	A	392	23.396	13.802	13.705	1.00	61.87	N
ATOM	3030	CA	LEU	A	392	24.325	13.561	12.625	1.00	59.99	C
ATOM	3031	CB	LEU	A	392	23.882	14.325	11.386	1.00	58.86	C
ATOM	3032	CG	LEU	A	392	23.834	13.519	10.102	1.00	57.12	C
ATOM	3033	CD1	LEU	A	392	22.900	12.340	10.305	1.00	52.74	C
ATOM	3034	CD2	LEU	A	392	23.386	14.412	8.960	1.00	52.71	C
ATOM	3035	C	LEU	A	392	25.711	14.007	13.014	1.00	61.46	C
ATOM	3036	O	LEU	A	392	26.672	13.662	12.343	1.00	67.20	O
ATOM	3037	N	ARG	A	393	25.809	14.806	14.072	1.00	60.61	N
ATOM	3038	CA	ARG	A	393	27.098	15.281	14.578	1.00	59.11	C
ATOM	3039	CB	ARG	A	393	26.847	16.421	15.565	1.00	60.33	C
ATOM	3040	CG	ARG	A	393	25.585	16.179	16.357	1.00	61.84	C
ATOM	3041	CD	ARG	A	393	25.321	17.199	17.437	1.00	67.54	C
ATOM	3042	NE	ARG	A	393	25.116	18.554	16.933	1.00	68.20	N
ATOM	3043	CZ	ARG	A	393	24.283	19.430	17.490	1.00	67.20	C
ATOM	3044	NH1	ARG	A	393	23.568	19.093	18.558	1.00	64.44	N
ATOM	3045	NH2	ARG	A	393	24.190	20.654	16.998	1.00	68.18	N
ATOM	3046	C	ARG	A	393	27.707	14.059	15.289	1.00	56.79	C
ATOM	3047	O	ARG	A	393	27.304	13.721	16.403	1.00	54.89	O
ATOM	3048	N	ASN	A	394	28.674	13.397	14.656	1.00	53.38	N
ATOM	3049	CA	ASN	A	394	29.221	12.199	15.256	1.00	50.59	C
ATOM	3050	CB	ASN	A	394	28.115	11.162	15.392	1.00	54.79	C
ATOM	3051	CG	ASN	A	394	27.780	10.851	16.819	1.00	61.68	C
ATOM	3052	OD1	ASN	A	394	27.321	11.717	17.571	1.00	66.61	O
ATOM	3053	ND2	ASN	A	394	28.000	9.601	17.212	1.00	64.19	N
ATOM	3054	C	ASN	A	394	30.371	11.526	14.532	1.00	49.03	C
ATOM	3055	O	ASN	A	394	30.460	10.310	14.568	1.00	55.63	O
ATOM	3056	N	GLY	A	395	31.238	12.268	13.863	1.00	42.93	N
ATOM	3057	CA	GLY	A	395	32.365	11.623	13.204	1.00	36.92	C
ATOM	3058	C	GLY	A	395	32.039	10.540	12.191	1.00	34.88	C
ATOM	3059	O	GLY	A	395	31.175	9.700	12.411	1.00	29.49	O
ATOM	3060	N	ALA	A	396	32.759	10.547	11.076	1.00	35.87	N
ATOM	3061	CA	ALA	A	396	32.520	9.592	10.007	1.00	38.03	C
ATOM	3062	CB	ALA	A	396	33.665	9.607	9.044	1.00	42.01	C
ATOM	3063	C	ALA	A	396	32.297	8.199	10.536	1.00	39.80	C
ATOM	3064	O	ALA	A	396	31.536	7.441	9.963	1.00	42.86	O
ATOM	3065	N	ASN	A	397	32.986	7.873	11.624	1.00	43.68	N
ATOM	3066	CA	ASN	A	397	32.881	6.584	12.316	1.00	45.05	C
ATOM	3067	CB	ASN	A	397	33.213	5.410	11.400	1.00	47.79	C
ATOM	3068	CG	ASN	A	397	34.635	5.444	10.908	1.00	53.12	C
ATOM	3069	OD1	ASN	A	397	35.178	4.431	10.458	1.00	56.78	O
ATOM	3070	ND2	ASN	A	397	35.249	6.613	10.980	1.00	53.42	N
ATOM	3071	C	ASN	A	397	33.847	6.586	13.493	1.00	45.39	C
ATOM	3072	O	ASN	A	397	34.733	7.449	13.576	1.00	40.24	O
ATOM	3073	N	GLU	A	398	33.663	5.624	14.400	1.00	47.70	N
ATOM	3074	CA	GLU	A	398	34.514	5.491	15.586	1.00	46.81	C
ATOM	3075	CB	GLU	A	398	34.248	4.157	16.293	1.00	44.98	C
ATOM	3076	CG	GLU	A	398	33.969	2.969	15.379	1.00	46.57	C
ATOM	3077	CD	GLU	A	398	33.702	1.679	16.154	1.00	48.98	C
ATOM	3078	OE1	GLU	A	398	32.796	1.668	17.009	1.00	48.26	O

345/396

Figure 3B-56

ATOM	3079	OE2	GLU	A	398	34.392	0.670	15.907	1.00	50.80	O
ATOM	3080	C	GLU	A	398	36.001	5.643	15.256	1.00	46.48	C
ATOM	3081	O	GLU	A	398	36.686	6.455	15.873	1.00	49.07	O
ATOM	3082	N	GLY	A	399	36.501	4.888	14.285	1.00	43.05	N
ATOM	3083	CA	GLY	A	399	37.896	5.038	13.922	1.00	44.45	C
ATOM	3084	C	GLY	A	399	38.291	6.510	13.900	1.00	45.91	C
ATOM	3085	O	GLY	A	399	39.164	6.951	14.648	1.00	43.90	O
ATOM	3086	N	PHE	A	400	37.619	7.272	13.043	1.00	47.00	N
ATOM	3087	CA	PHE	A	400	37.852	8.706	12.880	1.00	46.34	C
ATOM	3088	CB	PHE	A	400	36.722	9.317	12.046	1.00	47.22	C
ATOM	3089	CG	PHE	A	400	37.029	9.438	10.582	1.00	44.69	C
ATOM	3090	CD1	PHE	A	400	37.312	8.323	9.822	1.00	42.28	C
ATOM	3091	CD2	PHE	A	400	37.007	10.674	9.964	1.00	45.12	C
ATOM	3092	CE1	PHE	A	400	37.564	8.437	8.487	1.00	42.87	C
ATOM	3093	CE2	PHE	A	400	37.262	10.791	8.619	1.00	43.98	C
ATOM	3094	CZ	PHE	A	400	37.540	9.674	7.883	1.00	43.72	C
ATOM	3095	C	PHE	A	400	37.963	9.499	14.184	1.00	46.91	C
ATOM	3096	O	PHE	A	400	38.844	10.348	14.330	1.00	44.12	O
ATOM	3097	N	HIS	A	401	37.045	9.249	15.114	1.00	46.33	N
ATOM	3098	CA	HIS	A	401	37.043	9.963	16.383	1.00	46.79	C
ATOM	3099	CB	HIS	A	401	35.763	9.656	17.150	1.00	46.97	C
ATOM	3100	CG	HIS	A	401	35.037	10.877	17.632	1.00	49.37	C
ATOM	3101	CD2	HIS	A	401	33.736	11.238	17.529	1.00	47.28	C
ATOM	3102	ND1	HIS	A	401	35.654	11.874	18.357	1.00	48.25	N
ATOM	3103	CE1	HIS	A	401	34.764	12.794	18.682	1.00	47.01	C
ATOM	3104	NE2	HIS	A	401	33.594	12.431	18.193	1.00	48.71	N
ATOM	3105	C	HIS	A	401	38.251	9.552	17.210	1.00	48.28	C
ATOM	3106	O	HIS	A	401	39.011	10.394	17.711	1.00	49.43	O
ATOM	3107	N	GLU	A	402	38.425	8.242	17.343	1.00	46.56	N
ATOM	3108	CA	GLU	A	402	39.540	7.697	18.089	1.00	40.89	C
ATOM	3109	CB	GLU	A	402	39.382	6.191	18.256	1.00	35.78	C
ATOM	3110	CG	GLU	A	402	38.204	5.794	19.118	1.00	26.62	C
ATOM	3111	CD	GLU	A	402	38.292	6.408	20.505	1.00	29.50	C
ATOM	3112	OE1	GLU	A	402	39.330	7.058	20.826	1.00	17.63	O
ATOM	3113	OE2	GLU	A	402	37.324	6.233	21.278	1.00	29.14	O
ATOM	3114	C	GLU	A	402	40.817	7.975	17.349	1.00	40.83	C
ATOM	3115	O	GLU	A	402	41.880	7.908	17.917	1.00	45.05	O
ATOM	3116	N	ALA	A	403	40.713	8.310	16.077	1.00	43.09	N
ATOM	3117	CA	ALA	A	403	41.903	8.542	15.268	1.00	45.96	C
ATOM	3118	CB	ALA	A	403	41.683	7.959	13.861	1.00	40.95	C
ATOM	3119	C	ALA	A	403	42.348	9.983	15.148	1.00	46.32	C
ATOM	3120	O	ALA	A	403	43.285	10.280	14.411	1.00	46.17	O
ATOM	3121	N	VAL	A	404	41.719	10.886	15.879	1.00	48.00	N
ATOM	3122	CA	VAL	A	404	42.080	12.280	15.695	1.00	50.83	C
ATOM	3123	CB	VAL	A	404	40.786	13.184	15.715	1.00	50.21	C
ATOM	3124	CG1	VAL	A	404	40.055	13.038	17.031	1.00	51.65	C
ATOM	3125	CG2	VAL	A	404	41.133	14.624	15.431	1.00	45.19	C
ATOM	3126	C	VAL	A	404	43.141	12.775	16.648	1.00	51.98	C
ATOM	3127	O	VAL	A	404	44.079	13.436	16.238	1.00	50.40	O
ATOM	3128	N	GLY	A	405	43.006	12.447	17.922	1.00	59.46	N
ATOM	3129	CA	GLY	A	405	44.000	12.885	18.884	1.00	63.24	C
ATOM	3130	C	GLY	A	405	45.279	12.097	18.679	1.00	64.88	C
ATOM	3131	O	GLY	A	405	46.350	12.506	19.120	1.00	67.17	O
ATOM	3132	N	ALA	A	406	45.157	10.962	17.998	1.00	63.73	N
ATOM	3133	CA	ALA	A	406	46.290	10.097	17.724	1.00	62.60	C
ATOM	3134	CB	ALA	A	406	45.799	8.713	17.348	1.00	63.76	C

346/396

Figure 3B-57

ATOM	3135	C	ALA	A	406	47.107	10.686	16.591	1.00	63.60	C
ATOM	3136	O	ALA	A	406	48.252	10.311	16.378	1.00	64.31	O
ATOM	3137	N	ILE	A	407	46.501	11.606	15.854	1.00	65.82	N
ATOM	3138	CA	ILE	A	407	47.174	12.264	14.741	1.00	65.65	C
ATOM	3139	CB	ILE	A	407	46.157	12.827	13.736	1.00	64.86	C
ATOM	3140	CG2	ILE	A	407	46.847	13.775	12.769	1.00	61.23	C
ATOM	3141	CG1	ILE	A	407	45.466	11.665	13.014	1.00	66.89	C
ATOM	3142	CD1	ILE	A	407	44.314	12.068	12.112	1.00	68.62	C
ATOM	3143	C	ILE	A	407	48.010	13.399	15.290	1.00	67.06	C
ATOM	3144	O	ILE	A	407	48.942	13.875	14.639	1.00	68.91	O
ATOM	3145	N	MET	A	408	47.661	13.819	16.502	1.00	68.50	N
ATOM	3146	CA	MET	A	408	48.354	14.891	17.200	1.00	70.06	C
ATOM	3147	CB	MET	A	408	47.393	15.595	18.153	1.00	72.01	C
ATOM	3148	CG	MET	A	408	46.263	16.318	17.444	1.00	75.14	C
ATOM	3149	SD	MET	A	408	46.769	17.916	16.771	1.00	79.47	S
ATOM	3150	CE	MET	A	408	47.550	17.466	15.249	1.00	79.48	C
ATOM	3151	C	MET	A	408	49.532	14.318	17.973	1.00	70.07	C
ATOM	3152	O	MET	A	408	50.657	14.778	17.818	1.00	72.67	O
ATOM	3153	N	SER	A	409	49.276	13.312	18.801	1.00	67.71	N
ATOM	3154	CA	SER	A	409	50.340	12.684	19.570	1.00	66.48	C
ATOM	3155	CB	SER	A	409	49.807	11.455	20.297	1.00	66.04	C
ATOM	3156	OG	SER	A	409	48.870	11.821	21.292	1.00	70.67	O
ATOM	3157	C	SER	A	409	51.472	12.268	18.638	1.00	66.67	C
ATOM	3158	O	SER	A	409	52.645	12.498	18.917	1.00	67.80	O
ATOM	3159	N	LEU	A	410	51.105	11.664	17.517	1.00	65.57	N
ATOM	3160	CA	LEU	A	410	52.076	11.204	16.532	1.00	64.10	C
ATOM	3161	CB	LEU	A	410	51.346	10.802	15.242	1.00	57.19	C
ATOM	3162	CG	LEU	A	410	52.007	9.732	14.381	1.00	50.10	C
ATOM	3163	CD1	LEU	A	410	53.348	10.205	13.926	1.00	51.84	C
ATOM	3164	CD2	LEU	A	410	52.166	8.478	15.177	1.00	49.28	C
ATOM	3165	C	LEU	A	410	53.090	12.316	16.247	1.00	65.22	C
ATOM	3166	O	LEU	A	410	54.287	12.078	16.034	1.00	66.28	O
ATOM	3167	N	SER	A	411	52.597	13.541	16.258	1.00	64.49	N
ATOM	3168	CA	SER	A	411	53.436	14.688	15.996	1.00	66.73	C
ATOM	3169	CB	SER	A	411	52.583	15.765	15.310	1.00	68.77	C
ATOM	3170	OG	SER	A	411	53.231	17.021	15.265	1.00	72.29	O
ATOM	3171	C	SER	A	411	54.040	15.205	17.304	1.00	66.03	C
ATOM	3172	O	SER	A	411	55.250	15.429	17.407	1.00	65.08	O
ATOM	3173	N	ALA	A	412	53.183	15.375	18.303	1.00	65.17	N
ATOM	3174	CA	ALA	A	412	53.588	15.880	19.605	1.00	65.98	C
ATOM	3175	CB	ALA	A	412	52.401	16.572	20.279	1.00	67.64	C
ATOM	3176	C	ALA	A	412	54.135	14.779	20.505	1.00	64.50	C
ATOM	3177	O	ALA	A	412	53.588	14.505	21.575	1.00	65.30	O
ATOM	3178	N	ALA	A	413	55.218	14.156	20.055	1.00	62.13	N
ATOM	3179	CA	ALA	A	413	55.878	13.082	20.788	1.00	60.13	C
ATOM	3180	CB	ALA	A	413	55.044	11.808	20.747	1.00	58.42	C
ATOM	3181	C	ALA	A	413	57.205	12.861	20.097	1.00	59.39	C
ATOM	3182	O	ALA	A	413	58.097	12.196	20.611	1.00	61.12	O
ATOM	3183	N	THR	A	414	57.322	13.417	18.905	1.00	59.49	N
ATOM	3184	CA	THR	A	414	58.549	13.300	18.162	1.00	61.17	C
ATOM	3185	CB	THR	A	414	58.416	13.928	16.755	1.00	61.45	C
ATOM	3186	OG1	THR	A	414	57.886	15.258	16.857	1.00	56.85	O
ATOM	3187	CG2	THR	A	414	57.485	13.085	15.894	1.00	66.04	C
ATOM	3188	C	THR	A	414	59.566	14.079	18.969	1.00	64.08	C
ATOM	3189	O	THR	A	414	59.256	15.155	19.498	1.00	62.13	O
ATOM	3190	N	PRO	A	415	60.784	13.531	19.112	1.00	66.04	N

347/396

Figure 3B-58

ATOM	3191	CD	PRO	A	415	61.272	12.257	18.560	1.00	64.51	C
ATOM	3192	CA	PRO	A	415	61.837	14.207	19.866	1.00	67.05	C
ATOM	3193	CB	PRO	A	415	63.082	13.483	19.403	1.00	63.78	C
ATOM	3194	CG	PRO	A	415	62.586	12.085	19.282	1.00	64.27	C
ATOM	3195	C	PRO	A	415	61.806	15.663	19.440	1.00	70.55	C
ATOM	3196	O	PRO	A	415	61.825	16.572	20.264	1.00	71.73	O
ATOM	3197	N	LYS	A	416	61.737	15.863	18.130	1.00	74.68	N
ATOM	3198	CA	LYS	A	416	61.653	17.192	17.543	1.00	78.33	C
ATOM	3199	CB	LYS	A	416	61.076	17.086	16.126	1.00	80.48	C
ATOM	3200	CG	LYS	A	416	60.525	18.389	15.552	1.00	83.35	C
ATOM	3201	CD	LYS	A	416	61.528	19.103	14.656	1.00	83.41	C
ATOM	3202	CE	LYS	A	416	60.974	19.268	13.237	1.00	83.04	C
ATOM	3203	NZ	LYS	A	416	60.728	17.962	12.550	1.00	78.23	N
ATOM	3204	C	LYS	A	416	60.742	18.064	18.402	1.00	79.45	C
ATOM	3205	O	LYS	A	416	61.212	18.908	19.162	1.00	80.06	O
ATOM	3206	N	HIS	A	417	59.437	17.841	18.291	1.00	80.79	N
ATOM	3207	CA	HIS	A	417	58.479	18.621	19.050	1.00	81.37	C
ATOM	3208	CB	HIS	A	417	57.073	18.064	18.915	1.00	80.40	C
ATOM	3209	CG	HIS	A	417	56.054	18.882	19.635	1.00	81.55	C
ATOM	3210	CD2	HIS	A	417	55.289	18.609	20.718	1.00	82.17	C
ATOM	3211	ND1	HIS	A	417	55.767	20.185	19.282	1.00	80.82	N
ATOM	3212	CE1	HIS	A	417	54.870	20.677	20.115	1.00	81.39	C
ATOM	3213	NE2	HIS	A	417	54.563	19.741	20.997	1.00	82.53	N
ATOM	3214	C	HIS	A	417	58.824	18.653	20.517	1.00	82.48	C
ATOM	3215	O	HIS	A	417	59.091	19.715	21.076	1.00	82.75	O
ATOM	3216	N	LEU	A	418	58.808	17.477	21.138	1.00	84.17	N
ATOM	3217	CA	LEU	A	418	59.109	17.351	22.561	1.00	84.39	C
ATOM	3218	CB	LEU	A	418	59.396	15.886	22.915	1.00	83.44	C
ATOM	3219	CG	LEU	A	418	58.452	15.222	23.926	1.00	81.86	C
ATOM	3220	CD1	LEU	A	418	58.458	16.028	25.206	1.00	83.88	C
ATOM	3221	CD2	LEU	A	418	57.040	15.143	23.376	1.00	82.90	C
ATOM	3222	C	LEU	A	418	60.295	18.228	22.950	1.00	84.72	C
ATOM	3223	O	LEU	A	418	60.324	18.804	24.036	1.00	84.02	O
ATOM	3224	N	LYS	A	419	61.269	18.334	22.054	1.00	85.46	N
ATOM	3225	CA	LYS	A	419	62.447	19.147	22.315	1.00	86.53	C
ATOM	3226	CB	LYS	A	419	63.464	18.982	21.182	1.00	87.32	C
ATOM	3227	CG	LYS	A	419	64.769	19.751	21.370	1.00	88.93	C
ATOM	3228	CD	LYS	A	419	64.623	21.234	21.045	1.00	89.42	C
ATOM	3229	CE	LYS	A	419	65.983	21.908	21.014	1.00	90.58	C
ATOM	3230	NZ	LYS	A	419	66.938	21.173	20.132	1.00	88.29	N
ATOM	3231	C	LYS	A	419	62.038	20.604	22.444	1.00	86.92	C
ATOM	3232	O	LYS	A	419	62.137	21.191	23.516	1.00	87.35	O
ATOM	3233	N	SER	A	420	61.572	21.180	21.344	1.00	86.80	N
ATOM	3234	CA	SER	A	420	61.151	22.569	21.333	1.00	87.05	C
ATOM	3235	CB	SER	A	420	60.525	22.901	19.986	1.00	88.07	C
ATOM	3236	OG	SER	A	420	59.380	22.099	19.768	1.00	91.47	O
ATOM	3237	C	SER	A	420	60.153	22.884	22.444	1.00	86.71	C
ATOM	3238	O	SER	A	420	60.250	23.923	23.092	1.00	84.22	O
ATOM	3239	N	ILE	A	421	59.196	21.991	22.670	1.00	89.35	N
ATOM	3240	CA	ILE	A	421	58.197	22.234	23.705	1.00	92.25	C
ATOM	3241	CB	ILE	A	421	57.185	21.059	23.835	1.00	90.48	C
ATOM	3242	CG2	ILE	A	421	57.827	19.854	24.477	1.00	90.35	C
ATOM	3243	CG1	ILE	A	421	56.001	21.506	24.686	1.00	88.87	C
ATOM	3244	CD1	ILE	A	421	55.294	22.700	24.110	1.00	87.87	C
ATOM	3245	C	ILE	A	421	58.847	22.509	25.060	1.00	95.88	C
ATOM	3246	O	ILE	A	421	58.421	23.418	25.771	1.00	97.43	O

348/396

Figure 3B-59

ATOM	3247	N	GLY	A	422	59.878	21.739	25.417	1.00	98.67	N
ATOM	3248	CA	GLY	A	422	60.554	21.965	26.689	1.00	99.65	C
ATOM	3249	C	GLY	A	422	61.139	20.761	27.410	1.00	100.35	C
ATOM	3250	O	GLY	A	422	62.201	20.857	28.025	1.00	99.53	O
ATOM	3251	N	LEU	A	423	60.448	19.628	27.339	1.00	100.95	N
ATOM	3252	CA	LEU	A	423	60.889	18.409	28.006	1.00	100.84	C
ATOM	3253	CB	LEU	A	423	59.761	17.378	27.993	1.00	102.40	C
ATOM	3254	CG	LEU	A	423	58.418	17.850	28.557	1.00	105.96	C
ATOM	3255	CD1	LEU	A	423	57.362	16.768	28.381	1.00	105.72	C
ATOM	3256	CD2	LEU	A	423	58.585	18.206	30.026	1.00	107.11	C
ATOM	3257	C	LEU	A	423	62.125	17.799	27.366	1.00	100.65	C
ATOM	3258	O	LEU	A	423	62.298	16.583	27.395	1.00	99.39	O
ATOM	3259	N	LEU	A	424	62.992	18.630	26.800	1.00	101.94	N
ATOM	3260	CA	LEU	A	424	64.186	18.098	26.154	1.00	104.12	C
ATOM	3261	CB	LEU	A	424	63.755	17.180	25.006	1.00	99.27	C
ATOM	3262	CG	LEU	A	424	64.428	15.823	24.855	1.00	96.18	C
ATOM	3263	CD1	LEU	A	424	64.089	14.937	26.035	1.00	96.34	C
ATOM	3264	CD2	LEU	A	424	63.958	15.188	23.573	1.00	95.45	C
ATOM	3265	C	LEU	A	424	65.151	19.171	25.619	1.00	107.69	C
ATOM	3266	O	LEU	A	424	65.635	19.053	24.492	1.00	109.94	O
ATOM	3267	N	SER	A	425	65.437	20.200	26.420	1.00	110.32	N
ATOM	3268	CA	SER	A	425	66.343	21.288	26.016	1.00	111.24	C
ATOM	3269	CB	SER	A	425	66.855	22.027	27.260	1.00	112.04	C
ATOM	3270	OG	SER	A	425	67.349	21.124	28.235	1.00	114.42	O
ATOM	3271	C	SER	A	425	67.520	20.801	25.150	1.00	110.56	C
ATOM	3272	O	SER	A	425	68.074	19.724	25.395	1.00	108.93	O
ATOM	3273	N	PRO	A	426	67.936	21.619	24.156	1.00	110.08	N
ATOM	3274	CD	PRO	A	426	67.818	23.073	24.383	1.00	108.77	C
ATOM	3275	CA	PRO	A	426	69.020	21.364	23.196	1.00	110.17	C
ATOM	3276	CB	PRO	A	426	69.998	22.480	23.513	1.00	109.52	C
ATOM	3277	CG	PRO	A	426	69.052	23.643	23.652	1.00	108.91	C
ATOM	3278	C	PRO	A	426	69.632	19.963	23.260	1.00	110.18	C
ATOM	3279	O	PRO	A	426	70.644	19.741	23.926	1.00	109.67	O
ATOM	3280	N	ASP	A	427	69.014	19.029	22.535	1.00	110.39	N
ATOM	3281	CA	ASP	A	427	69.448	17.634	22.535	1.00	110.08	C
ATOM	3282	CB	ASP	A	427	68.229	16.704	22.644	1.00	110.32	C
ATOM	3283	CG	ASP	A	427	67.589	16.404	21.300	1.00	109.62	C
ATOM	3284	OD1	ASP	A	427	67.440	17.341	20.486	1.00	109.85	O
ATOM	3285	OD2	ASP	A	427	67.225	15.226	21.072	1.00	106.61	O
ATOM	3286	C	ASP	A	427	70.311	17.181	21.371	1.00	109.33	C
ATOM	3287	O	ASP	A	427	70.292	17.765	20.285	1.00	106.67	O
ATOM	3288	N	ALA	A	428	71.055	16.110	21.634	1.00	109.66	N
ATOM	3289	CA	ALA	A	428	71.966	15.503	20.676	1.00	109.87	C
ATOM	3290	CB	ALA	A	428	72.352	14.102	21.146	1.00	109.82	C
ATOM	3291	C	ALA	A	428	71.383	15.439	19.276	1.00	108.97	C
ATOM	3292	O	ALA	A	428	70.783	14.437	18.894	1.00	108.09	O
ATOM	3293	N	ALA	A	429	71.581	16.515	18.518	1.00	109.51	N
ATOM	3294	CA	ALA	A	429	71.093	16.614	17.147	1.00	109.71	C
ATOM	3295	CB	ALA	A	429	72.210	16.228	16.169	1.00	107.82	C
ATOM	3296	C	ALA	A	429	69.862	15.731	16.927	1.00	108.96	C
ATOM	3297	O	ALA	A	429	68.733	16.134	17.211	1.00	108.50	O
ATOM	3298	N	ALA	A	430	70.091	14.522	16.428	1.00	107.02	N
ATOM	3299	CA	ALA	A	430	69.006	13.594	16.174	1.00	105.71	C
ATOM	3300	CB	ALA	A	430	68.162	14.078	14.999	1.00	104.63	C
ATOM	3301	C	ALA	A	430	69.586	12.225	15.873	1.00	106.02	C
ATOM	3302	O	ALA	A	430	68.938	11.404	15.231	1.00	107.82	O

349/396

Figure 3B-60

ATOM	3303	N	ASP	A	431	70.811	11.998	16.338	1.00	105.42	N
ATOM	3304	CA	ASP	A	431	71.524	10.735	16.149	1.00	106.07	C
ATOM	3305	CB	ASP	A	431	71.940	10.152	17.501	1.00	111.14	C
ATOM	3306	CG	ASP	A	431	72.824	11.087	18.293	1.00	116.11	C
ATOM	3307	OD1	ASP	A	431	73.222	10.715	19.419	1.00	119.16	O
ATOM	3308	OD2	ASP	A	431	73.118	12.194	17.790	1.00	120.01	O
ATOM	3309	C	ASP	A	431	70.751	9.662	15.397	1.00	103.71	C
ATOM	3310	O	ASP	A	431	69.642	9.294	15.785	1.00	103.17	O
ATOM	3311	N	ASN	A	432	71.354	9.141	14.335	1.00	100.86	N
ATOM	3312	CA	ASN	A	432	70.726	8.089	13.548	1.00	97.89	C
ATOM	3313	CB	ASN	A	432	71.725	7.528	12.526	1.00	100.13	C
ATOM	3314	CG	ASN	A	432	72.934	6.857	13.183	1.00	102.20	C
ATOM	3315	OD1	ASN	A	432	73.773	6.265	12.503	1.00	104.07	O
ATOM	3316	ND2	ASN	A	432	73.027	6.951	14.504	1.00	101.32	N
ATOM	3317	C	ASN	A	432	70.266	6.972	14.485	1.00	94.33	C
ATOM	3318	O	ASN	A	432	69.530	6.069	14.083	1.00	92.45	O
ATOM	3319	N	GLU	A	433	70.698	7.057	15.742	1.00	91.25	N
ATOM	3320	CA	GLU	A	433	70.374	6.057	16.752	1.00	87.32	C
ATOM	3321	CB	GLU	A	433	71.612	5.744	17.583	1.00	87.92	C
ATOM	3322	CG	GLU	A	433	71.704	4.295	17.996	1.00	85.39	C
ATOM	3323	CD	GLU	A	433	72.807	4.057	18.982	1.00	83.70	C
ATOM	3324	OE1	GLU	A	433	72.638	4.461	20.152	1.00	81.93	O
ATOM	3325	OE2	GLU	A	433	73.838	3.476	18.585	1.00	81.87	O
ATOM	3326	C	GLU	A	433	69.236	6.446	17.684	1.00	84.48	C
ATOM	3327	O	GLU	A	433	68.476	5.587	18.132	1.00	84.06	O
ATOM	3328	N	THR	A	434	69.123	7.728	18.002	1.00	80.57	N
ATOM	3329	CA	THR	A	434	68.032	8.151	18.863	1.00	79.04	C
ATOM	3330	CB	THR	A	434	68.073	9.662	19.135	1.00	79.60	C
ATOM	3331	OG1	THR	A	434	67.984	10.369	17.894	1.00	80.01	O
ATOM	3332	CG2	THR	A	434	69.366	10.044	19.843	1.00	79.31	C
ATOM	3333	C	THR	A	434	66.741	7.818	18.123	1.00	77.50	C
ATOM	3334	O	THR	A	434	65.657	7.849	18.699	1.00	76.64	O
ATOM	3335	N	GLU	A	435	66.886	7.489	16.839	1.00	77.15	N
ATOM	3336	CA	GLU	A	435	65.775	7.137	15.953	1.00	76.09	C
ATOM	3337	CB	GLU	A	435	66.253	7.114	14.497	1.00	81.67	C
ATOM	3338	CG	GLU	A	435	65.455	7.995	13.523	1.00	88.07	C
ATOM	3339	CD	GLU	A	435	65.499	9.479	13.882	1.00	90.34	C
ATOM	3340	OE1	GLU	A	435	64.572	9.963	14.577	1.00	89.59	O
ATOM	3341	OE2	GLU	A	435	66.470	10.157	13.472	1.00	88.98	O
ATOM	3342	C	GLU	A	435	65.176	5.780	16.296	1.00	73.65	C
ATOM	3343	O	GLU	A	435	64.016	5.694	16.694	1.00	75.05	O
ATOM	3344	N	ILE	A	436	65.958	4.718	16.128	1.00	69.64	N
ATOM	3345	CA	ILE	A	436	65.477	3.378	16.439	1.00	66.68	C
ATOM	3346	CB	ILE	A	436	66.572	2.324	16.242	1.00	65.88	C
ATOM	3347	CG2	ILE	A	436	66.175	1.027	16.913	1.00	64.70	C
ATOM	3348	CG1	ILE	A	436	66.808	2.100	14.752	1.00	66.50	C
ATOM	3349	CD1	ILE	A	436	67.305	3.330	14.021	1.00	69.23	C
ATOM	3350	C	ILE	A	436	65.064	3.377	17.890	1.00	66.18	C
ATOM	3351	O	ILE	A	436	64.347	2.496	18.357	1.00	64.78	O
ATOM	3352	N	ASN	A	437	65.522	4.405	18.589	1.00	67.08	N
ATOM	3353	CA	ASN	A	437	65.251	4.582	20.000	1.00	67.64	C
ATOM	3354	CB	ASN	A	437	66.254	5.577	20.575	1.00	70.63	C
ATOM	3355	CG	ASN	A	437	66.844	5.111	21.880	1.00	71.86	C
ATOM	3356	OD1	ASN	A	437	67.191	3.933	22.025	1.00	68.37	O
ATOM	3357	ND2	ASN	A	437	66.975	6.031	22.838	1.00	68.50	N
ATOM	3358	C	ASN	A	437	63.840	5.087	20.209	1.00	65.71	C

350/396

Figure 3B-61

ATOM	3359	O	ASN	A 437	63.055	4.497	20.951	1.00	65.96	O
ATOM	3360	N	PHE	A 438	63.525	6.192	19.550	1.00	66.31	N
ATOM	3361	CA	PHE	A 438	62.198	6.797	19.645	1.00	67.79	C
ATOM	3362	CB	PHE	A 438	62.197	8.147	18.944	1.00	68.04	C
ATOM	3363	CG	PHE	A 438	60.892	8.489	18.316	1.00	71.78	C
ATOM	3364	CD1	PHE	A 438	59.768	8.690	19.093	1.00	73.40	C
ATOM	3365	CD2	PHE	A 438	60.786	8.611	16.942	1.00	72.53	C
ATOM	3366	CE1	PHE	A 438	58.555	9.009	18.508	1.00	75.01	C
ATOM	3367	CE2	PHE	A 438	59.581	8.927	16.357	1.00	73.19	C
ATOM	3368	CZ	PHE	A 438	58.463	9.127	17.141	1.00	73.53	C
ATOM	3369	C	PHE	A 438	61.141	5.906	19.009	1.00	65.63	C
ATOM	3370	O	PHE	A 438	60.084	5.657	19.588	1.00	62.68	O
ATOM	3371	N	LEU	A 439	61.457	5.437	17.806	1.00	62.76	N
ATOM	3372	CA	LEU	A 439	60.589	4.572	17.039	1.00	59.25	C
ATOM	3373	CB	LEU	A 439	61.234	4.301	15.684	1.00	57.73	C
ATOM	3374	CG	LEU	A 439	60.288	3.870	14.561	1.00	60.53	C
ATOM	3375	CD1	LEU	A 439	59.304	5.002	14.237	1.00	61.25	C
ATOM	3376	CD2	LEU	A 439	61.095	3.510	13.335	1.00	58.41	C
ATOM	3377	C	LEU	A 439	60.270	3.247	17.747	1.00	59.13	C
ATOM	3378	O	LEU	A 439	59.244	2.626	17.464	1.00	60.95	O
ATOM	3379	N	LEU	A 440	61.129	2.801	18.660	1.00	56.51	N
ATOM	3380	CA	LEU	A 440	60.854	1.545	19.354	1.00	54.29	C
ATOM	3381	CB	LEU	A 440	62.123	0.978	20.006	1.00	49.73	C
ATOM	3382	CG	LEU	A 440	62.086	-0.384	20.732	1.00	44.02	C
ATOM	3383	CD1	LEU	A 440	61.352	-0.256	22.030	1.00	41.36	C
ATOM	3384	CD2	LEU	A 440	61.437	-1.441	19.880	1.00	40.89	C
ATOM	3385	C	LEU	A 440	59.789	1.796	20.404	1.00	55.93	C
ATOM	3386	O	LEU	A 440	59.021	0.903	20.767	1.00	58.67	O
ATOM	3387	N	LYS	A 441	59.730	3.021	20.896	1.00	55.91	N
ATOM	3388	CA	LYS	A 441	58.726	3.339	21.896	1.00	55.10	C
ATOM	3389	CB	LYS	A 441	58.962	4.740	22.440	1.00	53.23	C
ATOM	3390	CG	LYS	A 441	58.269	4.987	23.728	1.00	45.88	C
ATOM	3391	CD	LYS	A 441	58.565	6.353	24.224	1.00	47.20	C
ATOM	3392	CE	LYS	A 441	57.551	6.649	25.260	1.00	54.15	C
ATOM	3393	NZ	LYS	A 441	57.147	5.325	25.800	1.00	55.57	N
ATOM	3394	C	LYS	A 441	57.356	3.244	21.225	1.00	56.38	C
ATOM	3395	O	LYS	A 441	56.511	2.444	21.634	1.00	55.10	O
ATOM	3396	N	GLN	A 442	57.158	4.061	20.188	1.00	56.34	N
ATOM	3397	CA	GLN	A 442	55.921	4.078	19.416	1.00	54.81	C
ATOM	3398	CB	GLN	A 442	56.150	4.721	18.059	1.00	56.80	C
ATOM	3399	CG	GLN	A 442	56.852	6.043	18.124	1.00	61.65	C
ATOM	3400	CD	GLN	A 442	56.032	7.076	18.841	1.00	63.14	C
ATOM	3401	OE1	GLN	A 442	55.519	8.010	18.225	1.00	64.80	O
ATOM	3402	NE2	GLN	A 442	55.891	6.913	20.154	1.00	62.54	N
ATOM	3403	C	GLN	A 442	55.472	2.657	19.180	1.00	54.51	C
ATOM	3404	O	GLN	A 442	54.373	2.270	19.576	1.00	54.68	O
ATOM	3405	N	ALA	A 443	56.336	1.885	18.526	1.00	53.81	N
ATOM	3406	CA	ALA	A 443	56.040	0.491	18.212	1.00	55.09	C
ATOM	3407	CB	ALA	A 443	57.304	-0.235	17.853	1.00	53.46	C
ATOM	3408	C	ALA	A 443	55.398	-0.154	19.420	1.00	56.00	C
ATOM	3409	O	ALA	A 443	54.362	-0.834	19.314	1.00	56.66	O
ATOM	3410	N	LEU	A 444	56.024	0.089	20.570	1.00	53.59	N
ATOM	3411	CA	LEU	A 444	55.562	-0.443	21.843	1.00	50.77	C
ATOM	3412	CB	LEU	A 444	56.458	0.082	22.977	1.00	50.07	C
ATOM	3413	CG	LEU	A 444	57.320	-0.874	23.820	1.00	45.61	C
ATOM	3414	CD1	LEU	A 444	57.674	-2.139	23.065	1.00	38.66	C

351/396

Figure 3B-62

ATOM	3415	CD2	LEU	A	444	58.566	-0.123	24.248	1.00	40.95	C
ATOM	3416	C	LEU	A	444	54.107	-0.052	22.068	1.00	47.21	C
ATOM	3417	O	LEU	A	444	53.287	-0.886	22.436	1.00	46.40	O
ATOM	3418	N	THR	A	445	53.789	1.212	21.823	1.00	44.96	N
ATOM	3419	CA	THR	A	445	52.430	1.703	22.004	1.00	45.87	C
ATOM	3420	CB	THR	A	445	52.422	3.224	22.180	1.00	41.97	C
ATOM	3421	OG1	THR	A	445	52.472	3.536	23.571	1.00	44.54	O
ATOM	3422	CG2	THR	A	445	51.188	3.823	21.593	1.00	39.42	C
ATOM	3423	C	THR	A	445	51.475	1.341	20.868	1.00	49.41	C
ATOM	3424	O	THR	A	445	50.422	0.728	21.091	1.00	51.58	O
ATOM	3425	N	ILE	A	446	51.851	1.702	19.646	1.00	49.53	N
ATOM	3426	CA	ILE	A	446	51.009	1.452	18.487	1.00	46.95	C
ATOM	3427	CB	ILE	A	446	51.403	2.388	17.355	1.00	43.52	C
ATOM	3428	CG2	ILE	A	446	50.444	2.270	16.213	1.00	39.52	C
ATOM	3429	CG1	ILE	A	446	51.384	3.819	17.882	1.00	46.46	C
ATOM	3430	CD1	ILE	A	446	52.178	4.812	17.040	1.00	49.59	C
ATOM	3431	C	ILE	A	446	50.976	0.015	17.978	1.00	49.06	C
ATOM	3432	O	ILE	A	446	49.887	-0.548	17.838	1.00	51.80	O
ATOM	3433	N	VAL	A	447	52.132	-0.595	17.710	1.00	46.85	N
ATOM	3434	CA	VAL	A	447	52.116	-1.969	17.197	1.00	43.36	C
ATOM	3435	CB	VAL	A	447	53.465	-2.448	16.661	1.00	43.51	C
ATOM	3436	CG1	VAL	A	447	53.272	-3.767	15.928	1.00	37.72	C
ATOM	3437	CG2	VAL	A	447	54.073	-1.421	15.748	1.00	46.82	C
ATOM	3438	C	VAL	A	447	51.745	-2.932	18.280	1.00	43.60	C
ATOM	3439	O	VAL	A	447	51.134	-3.970	18.019	1.00	42.47	O
ATOM	3440	N	GLY	A	448	52.132	-2.594	19.503	1.00	43.71	N
ATOM	3441	CA	GLY	A	448	51.824	-3.468	20.610	1.00	45.93	C
ATOM	3442	C	GLY	A	448	50.342	-3.761	20.668	1.00	47.98	C
ATOM	3443	O	GLY	A	448	49.916	-4.925	20.703	1.00	48.86	O
ATOM	3444	N	THR	A	449	49.559	-2.686	20.632	1.00	47.15	N
ATOM	3445	CA	THR	A	449	48.103	-2.756	20.732	1.00	44.85	C
ATOM	3446	CB	THR	A	449	47.551	-1.330	20.973	1.00	47.40	C
ATOM	3447	OG1	THR	A	449	46.549	-1.363	22.000	1.00	47.02	O
ATOM	3448	CG2	THR	A	449	46.963	-0.759	19.686	1.00	47.86	C
ATOM	3449	C	THR	A	449	47.292	-3.441	19.607	1.00	39.59	C
ATOM	3450	O	THR	A	449	46.264	-4.057	19.890	1.00	32.59	O
ATOM	3451	N	LEU	A	450	47.747	-3.349	18.355	1.00	35.27	N
ATOM	3452	CA	LEU	A	450	47.026	-3.939	17.222	1.00	34.26	C
ATOM	3453	CB	LEU	A	450	47.847	-3.817	15.958	1.00	30.62	C
ATOM	3454	CG	LEU	A	450	47.970	-2.389	15.426	1.00	38.23	C
ATOM	3455	CD1	LEU	A	450	49.031	-2.327	14.337	1.00	38.04	C
ATOM	3456	CD2	LEU	A	450	46.625	-1.931	14.879	1.00	37.83	C
ATOM	3457	C	LEU	A	450	46.583	-5.383	17.392	1.00	38.07	C
ATOM	3458	O	LEU	A	450	45.404	-5.702	17.260	1.00	35.74	O
ATOM	3459	N	PRO	A	451	47.524	-6.290	17.684	1.00	42.50	N
ATOM	3460	CD	PRO	A	451	48.971	-6.127	17.917	1.00	41.91	C
ATOM	3461	CA	PRO	A	451	47.122	-7.688	17.859	1.00	40.92	C
ATOM	3462	CB	PRO	A	451	48.455	-8.405	17.919	1.00	38.09	C
ATOM	3463	CG	PRO	A	451	49.314	-7.405	18.608	1.00	41.38	C
ATOM	3464	C	PRO	A	451	46.272	-7.857	19.124	1.00	41.45	C
ATOM	3465	O	PRO	A	451	45.387	-8.701	19.183	1.00	38.58	O
ATOM	3466	N	PHE	A	452	46.536	-7.032	20.130	1.00	45.01	N
ATOM	3467	CA	PHE	A	452	45.771	-7.080	21.377	1.00	47.07	C
ATOM	3468	CB	PHE	A	452	46.429	-6.194	22.452	1.00	50.95	C
ATOM	3469	CG	PHE	A	452	45.588	-6.023	23.691	1.00	53.25	C
ATOM	3470	CD1	PHE	A	452	44.552	-5.102	23.724	1.00	56.47	C

352/396

Figure 3B-63

ATOM	3471	CD2	PHE	A	452	45.770	-6.851	24.785	1.00	55.08	C
ATOM	3472	CE1	PHE	A	452	43.704	-5.014	24.821	1.00	56.41	C
ATOM	3473	CE2	PHE	A	452	44.930	-6.767	25.878	1.00	57.47	C
ATOM	3474	CZ	PHE	A	452	43.894	-5.845	25.892	1.00	55.93	C
ATOM	3475	C	PHE	A	452	44.369	-6.560	21.122	1.00	46.79	C
ATOM	3476	O	PHE	A	452	43.369	-7.106	21.621	1.00	42.54	O
ATOM	3477	N	THR	A	453	44.331	-5.470	20.355	1.00	46.54	N
ATOM	3478	CA	THR	A	453	43.107	-4.783	20.008	1.00	42.37	C
ATOM	3479	CB	THR	A	453	43.393	-3.471	19.327	1.00	44.87	C
ATOM	3480	OG1	THR	A	453	44.238	-2.677	20.169	1.00	43.31	O
ATOM	3481	CG2	THR	A	453	42.088	-2.738	19.069	1.00	48.17	C
ATOM	3482	C	THR	A	453	42.261	-5.606	19.096	1.00	38.57	C
ATOM	3483	O	THR	A	453	41.052	-5.602	19.220	1.00	38.96	O
ATOM	3484	N	TYR	A	454	42.903	-6.311	18.175	1.00	37.37	N
ATOM	3485	CA	TYR	A	454	42.196	-7.180	17.240	1.00	37.75	C
ATOM	3486	CB	TYR	A	454	43.163	-7.725	16.201	1.00	38.39	C
ATOM	3487	CG	TYR	A	454	42.604	-8.829	15.334	1.00	43.25	C
ATOM	3488	CD1	TYR	A	454	41.383	-9.429	15.619	1.00	44.76	C
ATOM	3489	CE1	TYR	A	454	40.879	-10.446	14.834	1.00	50.62	C
ATOM	3490	CD2	TYR	A	454	43.306	-9.283	14.228	1.00	46.97	C
ATOM	3491	CE2	TYR	A	454	42.805	-10.298	13.430	1.00	50.49	C
ATOM	3492	CZ	TYR	A	454	41.594	-10.874	13.739	1.00	50.65	C
ATOM	3493	OH	TYR	A	454	41.088	-11.873	12.947	1.00	54.69	O
ATOM	3494	C	TYR	A	454	41.561	-8.352	17.963	1.00	37.79	C
ATOM	3495	O	TYR	A	454	40.342	-8.476	18.022	1.00	38.09	O
ATOM	3496	N	MET	A	455	42.418	-9.224	18.485	1.00	38.94	N
ATOM	3497	CA	MET	A	455	42.016	-10.437	19.197	1.00	37.29	C
ATOM	3498	CB	MET	A	455	43.226	-11.000	19.947	1.00	36.50	C
ATOM	3499	CG	MET	A	455	43.055	-12.382	20.509	1.00	37.98	C
ATOM	3500	SD	MET	A	455	42.176	-12.416	22.084	1.00	49.46	S
ATOM	3501	CE	MET	A	455	43.419	-11.782	23.143	1.00	49.15	C
ATOM	3502	C	MET	A	455	40.828	-10.254	20.127	1.00	36.36	C
ATOM	3503	O	MET	A	455	39.873	-11.011	20.045	1.00	34.34	O
ATOM	3504	N	LEU	A	456	40.877	-9.239	20.988	1.00	40.54	N
ATOM	3505	CA	LEU	A	456	39.785	-8.969	21.923	1.00	45.68	C
ATOM	3506	CB	LEU	A	456	40.111	-7.743	22.803	1.00	45.38	C
ATOM	3507	CG	LEU	A	456	39.022	-7.278	23.790	1.00	41.98	C
ATOM	3508	CD1	LEU	A	456	39.597	-6.836	25.116	1.00	42.70	C
ATOM	3509	CD2	LEU	A	456	38.289	-6.129	23.172	1.00	45.86	C
ATOM	3510	C	LEU	A	456	38.451	-8.769	21.187	1.00	49.47	C
ATOM	3511	O	LEU	A	456	37.466	-9.451	21.495	1.00	49.48	O
ATOM	3512	N	GLU	A	457	38.410	-7.858	20.217	1.00	48.89	N
ATOM	3513	CA	GLU	A	457	37.172	-7.641	19.482	1.00	55.50	C
ATOM	3514	CB	GLU	A	457	37.337	-6.515	18.463	1.00	57.16	C
ATOM	3515	CG	GLU	A	457	36.968	-5.133	19.005	1.00	59.44	C
ATOM	3516	CD	GLU	A	457	35.465	-4.885	19.090	1.00	57.87	C
ATOM	3517	OE1	GLU	A	457	34.811	-4.819	18.029	1.00	54.34	O
ATOM	3518	OE2	GLU	A	457	34.942	-4.747	20.217	1.00	57.76	O
ATOM	3519	C	GLU	A	457	36.708	-8.908	18.769	1.00	59.07	C
ATOM	3520	O	GLU	A	457	35.506	-9.157	18.638	1.00	58.80	O
ATOM	3521	N	LYS	A	458	37.657	-9.707	18.293	1.00	63.79	N
ATOM	3522	CA	LYS	A	458	37.293	-10.935	17.609	1.00	65.45	C
ATOM	3523	CB	LYS	A	458	38.531	-11.693	17.127	1.00	65.77	C
ATOM	3524	CG	LYS	A	458	38.218	-13.026	16.429	1.00	69.85	C
ATOM	3525	CD	LYS	A	458	37.102	-12.891	15.375	1.00	71.01	C
ATOM	3526	CE	LYS	A	458	36.892	-14.182	14.554	1.00	68.74	C

353/396

Figure 3B-64

ATOM	3527	NZ	LYS	A	458	35.623	-14.187	13.762	1.00	58.48	N
ATOM	3528	C	LYS	A	458	36.517	-11.760	18.614	1.00	65.42	C
ATOM	3529	O	LYS	A	458	35.326	-11.989	18.434	1.00	68.45	O
ATOM	3530	N	TRP	A	459	37.178	-12.177	19.687	1.00	62.01	N
ATOM	3531	CA	TRP	A	459	36.508	-12.971	20.710	1.00	62.93	C
ATOM	3532	CB	TRP	A	459	37.397	-13.069	21.949	1.00	64.12	C
ATOM	3533	CG	TRP	A	459	36.848	-13.957	23.034	1.00	61.78	C
ATOM	3534	CD2	TRP	A	459	35.928	-13.575	24.061	1.00	59.52	C
ATOM	3535	CE2	TRP	A	459	35.697	-14.710	24.854	1.00	58.63	C
ATOM	3536	CE3	TRP	A	459	35.278	-12.380	24.385	1.00	58.99	C
ATOM	3537	CD1	TRP	A	459	37.128	-15.276	23.239	1.00	57.31	C
ATOM	3538	NE1	TRP	A	459	36.442	-15.735	24.333	1.00	55.22	N
ATOM	3539	CZ2	TRP	A	459	34.844	-14.685	25.957	1.00	60.24	C
ATOM	3540	CZ3	TRP	A	459	34.435	-12.359	25.479	1.00	59.04	C
ATOM	3541	CH2	TRP	A	459	34.225	-13.502	26.251	1.00	58.27	C
ATOM	3542	C	TRP	A	459	35.160	-12.340	21.086	1.00	63.38	C
ATOM	3543	O	TRP	A	459	34.166	-13.037	21.329	1.00	58.62	O
ATOM	3544	N	ARG	A	460	35.153	-11.008	21.126	1.00	65.81	N
ATOM	3545	CA	ARG	A	460	33.970	-10.204	21.457	1.00	63.85	C
ATOM	3546	CB	ARG	A	460	34.352	-8.718	21.453	1.00	63.63	C
ATOM	3547	CG	ARG	A	460	33.355	-7.786	22.081	1.00	60.88	C
ATOM	3548	CD	ARG	A	460	33.609	-7.672	23.552	1.00	61.58	C
ATOM	3549	NE	ARG	A	460	33.472	-6.294	24.000	1.00	62.32	N
ATOM	3550	CZ	ARG	A	460	34.136	-5.280	23.466	1.00	63.15	C
ATOM	3551	NH1	ARG	A	460	34.976	-5.491	22.472	1.00	61.21	N
ATOM	3552	NH2	ARG	A	460	33.959	-4.056	23.923	1.00	67.33	N
ATOM	3553	C	ARG	A	460	32.874	-10.465	20.419	1.00	60.54	C
ATOM	3554	O	ARG	A	460	31.690	-10.496	20.748	1.00	57.82	O
ATOM	3555	N	TRP	A	461	33.285	-10.634	19.164	1.00	58.78	N
ATOM	3556	CA	TRP	A	461	32.357	-10.926	18.072	1.00	59.63	C
ATOM	3557	CB	TRP	A	461	33.017	-10.694	16.713	1.00	56.87	C
ATOM	3558	CG	TRP	A	461	33.207	-9.263	16.311	1.00	54.45	C
ATOM	3559	CD2	TRP	A	461	34.301	-8.737	15.559	1.00	53.25	C
ATOM	3560	CE2	TRP	A	461	34.006	-7.394	15.272	1.00	54.26	C
ATOM	3561	CE3	TRP	A	461	35.504	-9.276	15.093	1.00	49.68	C
ATOM	3562	CD1	TRP	A	461	32.316	-8.236	16.457	1.00	51.80	C
ATOM	3563	NE1	TRP	A	461	32.785	-7.111	15.832	1.00	50.64	N
ATOM	3564	CZ2	TRP	A	461	34.871	-6.582	14.539	1.00	53.86	C
ATOM	3565	CZ3	TRP	A	461	36.358	-8.469	14.365	1.00	48.92	C
ATOM	3566	CH2	TRP	A	461	36.040	-7.142	14.096	1.00	51.02	C
ATOM	3567	C	TRP	A	461	31.918	-12.390	18.150	1.00	58.84	C
ATOM	3568	O	TRP	A	461	30.727	-12.698	18.139	1.00	59.01	O
ATOM	3569	N	MET	A	462	32.900	-13.279	18.223	1.00	56.96	N
ATOM	3570	CA	MET	A	462	32.669	-14.710	18.320	1.00	57.65	C
ATOM	3571	CB	MET	A	462	33.931	-15.395	18.818	1.00	59.04	C
ATOM	3572	CG	MET	A	462	35.184	-15.022	18.060	1.00	64.12	C
ATOM	3573	SD	MET	A	462	35.438	-16.039	16.622	1.00	66.86	S
ATOM	3574	CE	MET	A	462	36.156	-17.505	17.402	1.00	66.79	C
ATOM	3575	C	MET	A	462	31.547	-15.016	19.297	1.00	58.21	C
ATOM	3576	O	MET	A	462	30.624	-15.765	18.997	1.00	58.03	O
ATOM	3577	N	VAL	A	463	31.643	-14.437	20.482	1.00	59.14	N
ATOM	3578	CA	VAL	A	463	30.647	-14.665	21.513	1.00	60.14	C
ATOM	3579	CB	VAL	A	463	31.024	-13.912	22.787	1.00	58.77	C
ATOM	3580	CG1	VAL	A	463	29.991	-14.154	23.861	1.00	57.55	C
ATOM	3581	CG2	VAL	A	463	32.396	-14.367	23.252	1.00	59.01	C
ATOM	3582	C	VAL	A	463	29.244	-14.260	21.080	1.00	61.80	C

354/396

Figure 3B-65

ATOM	3583	O	VAL	A	463	28.318	-15.079	21.090	1.00	61.31	O
ATOM	3584	N	PHE	A	464	29.085	-12.996	20.709	1.00	63.40	N
ATOM	3585	CA	PHE	A	464	27.787	-12.504	20.270	1.00	66.70	C
ATOM	3586	CB	PHE	A	464	27.910	-11.052	19.800	1.00	69.09	C
ATOM	3587	CG	PHE	A	464	28.333	-10.092	20.884	1.00	69.33	C
ATOM	3588	CD1	PHE	A	464	28.814	-8.839	20.567	1.00	68.78	C
ATOM	3589	CD2	PHE	A	464	28.234	-10.437	22.219	1.00	68.79	C
ATOM	3590	CE1	PHE	A	464	29.187	-7.954	21.559	1.00	66.75	C
ATOM	3591	CE2	PHE	A	464	28.607	-9.548	23.208	1.00	65.59	C
ATOM	3592	CZ	PHE	A	464	29.081	-8.312	22.876	1.00	62.38	C
ATOM	3593	C	PHE	A	464	27.318	-13.396	19.126	1.00	67.55	C
ATOM	3594	O	PHE	A	464	26.173	-13.836	19.097	1.00	67.54	O
ATOM	3595	N	LYS	A	465	28.230	-13.658	18.192	1.00	68.02	N
ATOM	3596	CA	LYS	A	465	27.975	-14.508	17.034	1.00	67.46	C
ATOM	3597	CB	LYS	A	465	29.282	-14.773	16.304	1.00	68.73	C
ATOM	3598	CG	LYS	A	465	29.136	-15.352	14.930	1.00	72.37	C
ATOM	3599	CD	LYS	A	465	29.997	-14.555	13.955	1.00	74.80	C
ATOM	3600	CE	LYS	A	465	29.575	-13.083	13.931	1.00	73.97	C
ATOM	3601	NZ	LYS	A	465	30.413	-12.285	12.997	1.00	73.45	N
ATOM	3602	C	LYS	A	465	27.432	-15.813	17.556	1.00	68.98	C
ATOM	3603	O	LYS	A	465	26.302	-16.180	17.270	1.00	70.22	O
ATOM	3604	N	GLY	A	466	28.256	-16.507	18.335	1.00	71.20	N
ATOM	3605	CA	GLY	A	466	27.854	-17.772	18.924	1.00	72.35	C
ATOM	3606	C	GLY	A	466	28.963	-18.808	18.925	1.00	73.10	C
ATOM	3607	O	GLY	A	466	28.936	-19.771	19.701	1.00	73.10	O
ATOM	3608	N	GLU	A	467	29.950	-18.594	18.061	1.00	71.94	N
ATOM	3609	CA	GLU	A	467	31.077	-19.505	17.906	1.00	71.95	C
ATOM	3610	CB	GLU	A	467	32.091	-18.893	16.940	1.00	74.48	C
ATOM	3611	CG	GLU	A	467	31.466	-18.009	15.871	1.00	76.16	C
ATOM	3612	CD	GLU	A	467	32.440	-17.668	14.760	1.00	78.41	C
ATOM	3613	OE1	GLU	A	467	33.580	-17.256	15.063	1.00	77.04	O
ATOM	3614	OE2	GLU	A	467	32.063	-17.809	13.577	1.00	81.52	O
ATOM	3615	C	GLU	A	467	31.782	-19.891	19.204	1.00	70.95	C
ATOM	3616	O	GLU	A	467	32.765	-20.628	19.185	1.00	68.26	O
ATOM	3617	N	ILE	A	468	31.288	-19.385	20.325	1.00	72.32	N
ATOM	3618	CA	ILE	A	468	31.881	-19.680	21.624	1.00	76.32	C
ATOM	3619	CB	ILE	A	468	32.898	-18.578	22.054	1.00	72.67	C
ATOM	3620	CG2	ILE	A	468	33.715	-19.047	23.246	1.00	70.83	C
ATOM	3621	CG1	ILE	A	468	33.865	-18.277	20.915	1.00	68.36	C
ATOM	3622	CD1	ILE	A	468	34.947	-17.333	21.300	1.00	66.15	C
ATOM	3623	C	ILE	A	468	30.777	-19.783	22.682	1.00	81.34	C
ATOM	3624	O	ILE	A	468	30.264	-18.771	23.176	1.00	81.95	O
ATOM	3625	N	PRO	A	469	30.395	-21.020	23.037	1.00	84.55	N
ATOM	3626	CD	PRO	A	469	31.011	-22.260	22.529	1.00	85.58	C
ATOM	3627	CA	PRO	A	469	29.358	-21.320	24.030	1.00	84.61	C
ATOM	3628	CB	PRO	A	469	29.133	-22.810	23.839	1.00	86.80	C
ATOM	3629	CG	PRO	A	469	30.526	-23.296	23.516	1.00	86.32	C
ATOM	3630	C	PRO	A	469	29.834	-20.973	25.435	1.00	84.46	C
ATOM	3631	O	PRO	A	469	30.978	-21.247	25.805	1.00	82.29	O
ATOM	3632	N	LYS	A	470	28.942	-20.373	26.210	1.00	84.93	N
ATOM	3633	CA	LYS	A	470	29.252	-19.946	27.564	1.00	85.72	C
ATOM	3634	CB	LYS	A	470	27.973	-19.917	28.400	1.00	86.15	C
ATOM	3635	CG	LYS	A	470	26.945	-18.928	27.849	1.00	89.47	C
ATOM	3636	CD	LYS	A	470	25.805	-18.638	28.821	1.00	89.65	C
ATOM	3637	CE	LYS	A	470	24.928	-17.506	28.293	1.00	89.04	C
ATOM	3638	NZ	LYS	A	470	25.727	-16.282	27.984	1.00	84.22	N

355/396

Figure 3B-66

ATOM	3639	C	LYS	A	470	30.325	-20.752	28.270	1.00	86.18	C
ATOM	3640	O	LYS	A	470	31.215	-20.180	28.885	1.00	86.79	O
ATOM	3641	N	ASP	A	471	30.259	-22.073	28.165	1.00	89.40	N
ATOM	3642	CA	ASP	A	471	31.231	-22.936	28.832	1.00	91.52	C
ATOM	3643	CB	ASP	A	471	30.704	-24.378	28.933	1.00	95.41	C
ATOM	3644	CG	ASP	A	471	30.300	-24.966	27.579	1.00	98.56	C
ATOM	3645	OD1	ASP	A	471	29.126	-24.791	27.172	1.00	98.34	O
ATOM	3646	OD2	ASP	A	471	31.159	-25.604	26.925	1.00	98.02	O
ATOM	3647	C	ASP	A	471	32.613	-22.960	28.201	1.00	91.10	C
ATOM	3648	O	ASP	A	471	33.493	-23.685	28.665	1.00	91.12	O
ATOM	3649	N	GLN	A	472	32.816	-22.167	27.156	1.00	91.44	N
ATOM	3650	CA	GLN	A	472	34.113	-22.140	26.489	1.00	91.78	C
ATOM	3651	CB	GLN	A	472	34.008	-22.828	25.123	1.00	95.51	C
ATOM	3652	CG	GLN	A	472	33.508	-24.271	25.177	1.00	98.63	C
ATOM	3653	CD	GLN	A	472	34.401	-25.180	26.006	1.00	100.37	C
ATOM	3654	OE1	GLN	A	472	35.584	-25.359	25.702	1.00	101.74	O
ATOM	3655	NE2	GLN	A	472	33.836	-25.763	27.058	1.00	100.27	N
ATOM	3656	C	GLN	A	472	34.669	-20.727	26.312	1.00	89.06	C
ATOM	3657	O	GLN	A	472	35.517	-20.490	25.454	1.00	89.55	O
ATOM	3658	N	TRP	A	473	34.198	-19.795	27.130	1.00	85.44	N
ATOM	3659	CA	TRP	A	473	34.651	-18.416	27.044	1.00	81.50	C
ATOM	3660	CB	TRP	A	473	33.790	-17.528	27.936	1.00	79.55	C
ATOM	3661	CG	TRP	A	473	32.481	-17.193	27.340	1.00	75.51	C
ATOM	3662	CD2	TRP	A	473	31.526	-16.258	27.844	1.00	75.26	C
ATOM	3663	CE2	TRP	A	473	30.409	-16.301	26.987	1.00	76.92	C
ATOM	3664	CE3	TRP	A	473	31.505	-15.385	28.936	1.00	75.22	C
ATOM	3665	CD1	TRP	A	473	31.929	-17.747	26.232	1.00	75.67	C
ATOM	3666	NE1	TRP	A	473	30.683	-17.220	26.009	1.00	76.56	N
ATOM	3667	CZ2	TRP	A	473	29.275	-15.510	27.189	1.00	78.30	C
ATOM	3668	CZ3	TRP	A	473	30.381	-14.599	29.139	1.00	78.35	C
ATOM	3669	CH2	TRP	A	473	29.281	-14.665	28.267	1.00	79.87	C
ATOM	3670	C	TRP	A	473	36.119	-18.224	27.404	1.00	81.15	C
ATOM	3671	O	TRP	A	473	36.896	-17.695	26.604	1.00	80.10	O
ATOM	3672	N	MET	A	474	36.501	-18.638	28.608	1.00	80.45	N
ATOM	3673	CA	MET	A	474	37.887	-18.482	29.035	1.00	80.84	C
ATOM	3674	CB	MET	A	474	37.997	-18.669	30.543	1.00	80.66	C
ATOM	3675	CG	MET	A	474	37.178	-17.639	31.285	1.00	81.70	C
ATOM	3676	SD	MET	A	474	37.372	-16.007	30.515	1.00	79.47	S
ATOM	3677	CE	MET	A	474	38.851	-15.432	31.330	1.00	82.89	C
ATOM	3678	C	MET	A	474	38.785	-19.454	28.295	1.00	80.62	C
ATOM	3679	O	MET	A	474	40.013	-19.416	28.419	1.00	79.48	O
ATOM	3680	N	LYS	A	475	38.143	-20.321	27.519	1.00	80.45	N
ATOM	3681	CA	LYS	A	475	38.831	-21.298	26.696	1.00	79.78	C
ATOM	3682	CB	LYS	A	475	37.835	-22.330	26.166	1.00	80.04	C
ATOM	3683	CG	LYS	A	475	37.715	-23.582	27.012	1.00	83.38	C
ATOM	3684	CD	LYS	A	475	38.944	-24.469	26.860	1.00	83.95	C
ATOM	3685	CE	LYS	A	475	39.068	-24.997	25.433	1.00	84.98	C
ATOM	3686	NZ	LYS	A	475	40.302	-25.816	25.250	1.00	85.57	N
ATOM	3687	C	LYS	A	475	39.451	-20.535	25.529	1.00	79.18	C
ATOM	3688	O	LYS	A	475	40.621	-20.147	25.583	1.00	81.25	O
ATOM	3689	N	LYS	A	476	38.648	-20.302	24.491	1.00	75.27	N
ATOM	3690	CA	LYS	A	476	39.101	-19.588	23.302	1.00	70.88	C
ATOM	3691	CB	LYS	A	476	37.916	-19.120	22.445	1.00	73.42	C
ATOM	3692	CG	LYS	A	476	37.134	-20.213	21.721	1.00	74.93	C
ATOM	3693	CD	LYS	A	476	37.949	-20.896	20.626	1.00	72.24	C
ATOM	3694	CE	LYS	A	476	37.089	-21.922	19.906	1.00	74.43	C

356/396

Figure 3B-67

ATOM	3695	NZ	LYS	A	476	36.230	-22.701	20.860	1.00	73.93	N
ATOM	3696	C	LYS	A	476	39.914	-18.371	23.669	1.00	67.73	C
ATOM	3697	O	LYS	A	476	40.884	-18.050	22.996	1.00	66.93	O
ATOM	3698	N	TRP	A	477	39.521	-17.697	24.744	1.00	65.81	N
ATOM	3699	CA	TRP	A	477	40.206	-16.481	25.158	1.00	62.97	C
ATOM	3700	CB	TRP	A	477	39.585	-15.924	26.444	1.00	64.42	C
ATOM	3701	CG	TRP	A	477	40.214	-14.624	26.849	1.00	67.81	C
ATOM	3702	CD2	TRP	A	477	40.002	-13.347	26.238	1.00	70.12	C
ATOM	3703	CE2	TRP	A	477	40.862	-12.429	26.878	1.00	72.02	C
ATOM	3704	CE3	TRP	A	477	39.173	-12.889	25.211	1.00	68.48	C
ATOM	3705	CD1	TRP	A	477	41.166	-14.433	27.812	1.00	67.08	C
ATOM	3706	NE1	TRP	A	477	41.561	-13.121	27.836	1.00	69.71	N
ATOM	3707	CZ2	TRP	A	477	40.916	-11.081	26.524	1.00	70.07	C
ATOM	3708	CZ3	TRP	A	477	39.229	-11.557	24.863	1.00	71.25	C
ATOM	3709	CH2	TRP	A	477	40.093	-10.668	25.518	1.00	70.63	C
ATOM	3710	C	TRP	A	477	41.716	-16.609	25.320	1.00	59.14	C
ATOM	3711	O	TRP	A	477	42.477	-15.733	24.899	1.00	56.98	O
ATOM	3712	N	TRP	A	478	42.164	-17.701	25.916	1.00	56.06	N
ATOM	3713	CA	TRP	A	478	43.590	-17.863	26.105	1.00	53.98	C
ATOM	3714	CB	TRP	A	478	43.848	-18.503	27.450	1.00	50.65	C
ATOM	3715	CG	TRP	A	478	43.545	-17.550	28.553	1.00	40.50	C
ATOM	3716	CD2	TRP	A	478	44.354	-16.437	28.957	1.00	35.32	C
ATOM	3717	CE2	TRP	A	478	43.693	-15.811	30.021	1.00	33.05	C
ATOM	3718	CE3	TRP	A	478	45.578	-15.915	28.518	1.00	35.02	C
ATOM	3719	CD1	TRP	A	478	42.451	-17.549	29.360	1.00	32.39	C
ATOM	3720	NE1	TRP	A	478	42.532	-16.505	30.247	1.00	33.86	N
ATOM	3721	CZ2	TRP	A	478	44.210	-14.690	30.659	1.00	32.95	C
ATOM	3722	CZ3	TRP	A	478	46.090	-14.801	29.146	1.00	32.18	C
ATOM	3723	CH2	TRP	A	478	45.408	-14.201	30.206	1.00	35.47	C
ATOM	3724	C	TRP	A	478	44.242	-18.636	24.986	1.00	55.99	C
ATOM	3725	O	TRP	A	478	45.425	-18.447	24.701	1.00	57.05	O
ATOM	3726	N	GLU	A	479	43.461	-19.509	24.357	1.00	58.47	N
ATOM	3727	CA	GLU	A	479	43.922	-20.273	23.207	1.00	60.25	C
ATOM	3728	CB	GLU	A	479	42.746	-21.044	22.610	1.00	60.24	C
ATOM	3729	CG	GLU	A	479	43.016	-22.505	22.306	1.00	67.69	C
ATOM	3730	CD	GLU	A	479	41.890	-23.423	22.791	1.00	71.45	C
ATOM	3731	OE1	GLU	A	479	40.700	-23.094	22.557	1.00	68.16	O
ATOM	3732	OE2	GLU	A	479	42.205	-24.477	23.401	1.00	71.77	O
ATOM	3733	C	GLU	A	479	44.345	-19.145	22.264	1.00	63.25	C
ATOM	3734	O	GLU	A	479	45.477	-19.128	21.748	1.00	63.08	O
ATOM	3735	N	MET	A	480	43.415	-18.189	22.100	1.00	63.54	N
ATOM	3736	CA	MET	A	480	43.561	-16.982	21.274	1.00	60.26	C
ATOM	3737	CB	MET	A	480	42.274	-16.171	21.285	1.00	54.69	C
ATOM	3738	CG	MET	A	480	41.117	-16.800	20.602	1.00	54.87	C
ATOM	3739	SD	MET	A	480	39.750	-15.640	20.505	1.00	55.23	S
ATOM	3740	CE	MET	A	480	40.179	-14.811	19.012	1.00	52.81	C
ATOM	3741	C	MET	A	480	44.671	-16.053	21.754	1.00	60.65	C
ATOM	3742	O	MET	A	480	45.549	-15.653	20.988	1.00	59.82	O
ATOM	3743	N	LYS	A	481	44.603	-15.664	23.017	1.00	59.83	N
ATOM	3744	CA	LYS	A	481	45.628	-14.789	23.542	1.00	64.57	C
ATOM	3745	CB	LYS	A	481	45.521	-14.708	25.069	1.00	63.96	C
ATOM	3746	CG	LYS	A	481	45.038	-13.374	25.618	1.00	60.12	C
ATOM	3747	CD	LYS	A	481	46.056	-12.275	25.385	1.00	59.45	C
ATOM	3748	CE	LYS	A	481	45.559	-10.941	25.945	1.00	65.19	C
ATOM	3749	NZ	LYS	A	481	44.208	-10.522	25.434	1.00	63.63	N
ATOM	3750	C	LYS	A	481	46.970	-15.389	23.135	1.00	68.21	C

357/396

Figure 3B-68

ATOM	3751	O	LYS	A	481	47.952	-14.665	22.938	1.00	68.16	O
ATOM	3752	N	ARG	A	482	46.986	-16.718	22.984	1.00	71.36	N
ATOM	3753	CA	ARG	A	482	48.197	-17.460	22.629	1.00	74.43	C
ATOM	3754	CB	ARG	A	482	48.127	-18.884	23.202	1.00	76.01	C
ATOM	3755	CG	ARG	A	482	48.944	-19.026	24.487	1.00	79.83	C
ATOM	3756	CD	ARG	A	482	48.796	-20.376	25.184	1.00	84.45	C
ATOM	3757	NE	ARG	A	482	47.442	-20.605	25.689	1.00	88.91	N
ATOM	3758	CZ	ARG	A	482	47.148	-21.369	26.739	1.00	88.54	C
ATOM	3759	NH1	ARG	A	482	48.117	-21.982	27.410	1.00	88.35	N
ATOM	3760	NH2	ARG	A	482	45.884	-21.522	27.115	1.00	86.29	N
ATOM	3761	C	ARG	A	482	48.600	-17.506	21.156	1.00	73.40	C
ATOM	3762	O	ARG	A	482	49.771	-17.313	20.840	1.00	74.80	O
ATOM	3763	N	GLU	A	483	47.666	-17.769	20.250	1.00	72.25	N
ATOM	3764	CA	GLU	A	483	48.029	-17.793	18.833	1.00	73.12	C
ATOM	3765	CB	GLU	A	483	46.946	-18.457	17.988	1.00	75.52	C
ATOM	3766	CG	GLU	A	483	46.773	-19.930	18.213	1.00	82.86	C
ATOM	3767	CD	GLU	A	483	45.699	-20.508	17.316	1.00	87.45	C
ATOM	3768	OE1	GLU	A	483	44.557	-19.998	17.348	1.00	90.01	O
ATOM	3769	OE2	GLU	A	483	45.995	-21.472	16.578	1.00	90.42	O
ATOM	3770	C	GLU	A	483	48.239	-16.380	18.303	1.00	71.12	C
ATOM	3771	O	GLU	A	483	49.349	-16.007	17.930	1.00	69.99	O
ATOM	3772	N	ILE	A	484	47.146	-15.613	18.290	1.00	70.61	N
ATOM	3773	CA	ILE	A	484	47.092	-14.232	17.801	1.00	65.37	C
ATOM	3774	CB	ILE	A	484	45.644	-13.729	17.798	1.00	64.74	C
ATOM	3775	CG2	ILE	A	484	45.509	-12.551	16.847	1.00	67.12	C
ATOM	3776	CG1	ILE	A	484	44.704	-14.852	17.365	1.00	61.97	C
ATOM	3777	CD1	ILE	A	484	43.256	-14.427	17.284	1.00	62.51	C
ATOM	3778	C	ILE	A	484	47.936	-13.203	18.555	1.00	63.24	C
ATOM	3779	O	ILE	A	484	48.945	-12.739	18.044	1.00	62.39	O
ATOM	3780	N	VAL	A	485	47.529	-12.833	19.764	1.00	62.42	N
ATOM	3781	CA	VAL	A	485	48.298	-11.835	20.499	1.00	62.56	C
ATOM	3782	CB	VAL	A	485	47.695	-11.506	21.868	1.00	62.14	C
ATOM	3783	CG1	VAL	A	485	48.540	-10.426	22.532	1.00	59.88	C
ATOM	3784	CG2	VAL	A	485	46.254	-11.044	21.718	1.00	60.53	C
ATOM	3785	C	VAL	A	485	49.713	-12.294	20.748	1.00	62.76	C
ATOM	3786	O	VAL	A	485	50.659	-11.517	20.646	1.00	59.48	O
ATOM	3787	N	GLY	A	486	49.843	-13.570	21.084	1.00	67.10	N
ATOM	3788	CA	GLY	A	486	51.144	-14.139	21.370	1.00	69.55	C
ATOM	3789	C	GLY	A	486	51.427	-13.901	22.833	1.00	71.58	C
ATOM	3790	O	GLY	A	486	52.494	-13.396	23.189	1.00	74.36	O
ATOM	3791	N	VAL	A	487	50.465	-14.267	23.679	1.00	70.01	N
ATOM	3792	CA	VAL	A	487	50.590	-14.083	25.121	1.00	68.46	C
ATOM	3793	CB	VAL	A	487	49.922	-12.748	25.555	1.00	68.23	C
ATOM	3794	CG1	VAL	A	487	49.176	-12.919	26.858	1.00	68.90	C
ATOM	3795	CG2	VAL	A	487	50.984	-11.673	25.710	1.00	65.56	C
ATOM	3796	C	VAL	A	487	49.976	-15.259	25.880	1.00	68.81	C
ATOM	3797	O	VAL	A	487	49.014	-15.872	25.412	1.00	65.83	O
ATOM	3798	N	VAL	A	488	50.549	-15.577	27.045	1.00	69.46	N
ATOM	3799	CA	VAL	A	488	50.071	-16.692	27.868	1.00	67.74	C
ATOM	3800	CB	VAL	A	488	51.117	-17.839	27.927	1.00	66.60	C
ATOM	3801	CG1	VAL	A	488	52.275	-17.438	28.821	1.00	68.04	C
ATOM	3802	CG2	VAL	A	488	50.464	-19.126	28.416	1.00	64.60	C
ATOM	3803	C	VAL	A	488	49.742	-16.258	29.292	1.00	65.81	C
ATOM	3804	O	VAL	A	488	50.329	-15.306	29.817	1.00	64.01	O
ATOM	3805	N	GLU	A	489	48.815	-16.987	29.908	1.00	64.18	N
ATOM	3806	CA	GLU	A	489	48.347	-16.715	31.259	1.00	67.48	C

358/396

Figure 3B-69

ATOM	3807	CB	GLU	A	489	46.891	-17.163	31.391	1.00	65.17	C
ATOM	3808	CG	GLU	A	489	46.637	-18.659	31.293	1.00	66.18	C
ATOM	3809	CD	GLU	A	489	46.802	-19.221	29.892	1.00	68.85	C
ATOM	3810	OE1	GLU	A	489	46.108	-20.215	29.573	1.00	67.01	O
ATOM	3811	OE2	GLU	A	489	47.624	-18.689	29.115	1.00	67.68	O
ATOM	3812	C	GLU	A	489	49.163	-17.337	32.390	1.00	70.73	C
ATOM	3813	O	GLU	A	489	49.379	-18.541	32.407	1.00	72.76	O
ATOM	3814	N	PRO	A	490	49.627	-16.510	33.351	1.00	74.09	N
ATOM	3815	CD	PRO	A	490	49.673	-15.048	33.176	1.00	76.91	C
ATOM	3816	CA	PRO	A	490	50.425	-16.898	34.526	1.00	75.88	C
ATOM	3817	CB	PRO	A	490	50.752	-15.559	35.184	1.00	75.05	C
ATOM	3818	CG	PRO	A	490	50.878	-14.657	34.014	1.00	76.72	C
ATOM	3819	C	PRO	A	490	49.706	-17.831	35.491	1.00	75.77	C
ATOM	3820	O	PRO	A	490	50.286	-18.252	36.492	1.00	78.63	O
ATOM	3821	N	VAL	A	491	48.449	-18.146	35.194	1.00	72.57	N
ATOM	3822	CA	VAL	A	491	47.654	-19.026	36.041	1.00	71.69	C
ATOM	3823	CB	VAL	A	491	47.077	-18.272	37.258	1.00	69.93	C
ATOM	3824	CG1	VAL	A	491	46.270	-19.226	38.114	1.00	70.41	C
ATOM	3825	CG2	VAL	A	491	48.191	-17.635	38.077	1.00	67.25	C
ATOM	3826	C	VAL	A	491	46.482	-19.576	35.243	1.00	72.83	C
ATOM	3827	O	VAL	A	491	45.933	-18.892	34.397	1.00	76.51	O
ATOM	3828	N	PRO	A	492	46.084	-20.824	35.494	1.00	73.75	N
ATOM	3829	CD	PRO	A	492	46.795	-21.926	36.155	1.00	76.33	C
ATOM	3830	CA	PRO	A	492	44.953	-21.336	34.722	1.00	74.05	C
ATOM	3831	CB	PRO	A	492	44.970	-22.827	35.028	1.00	74.35	C
ATOM	3832	CG	PRO	A	492	46.408	-23.099	35.282	1.00	77.59	C
ATOM	3833	C	PRO	A	492	43.666	-20.681	35.192	1.00	75.34	C
ATOM	3834	O	PRO	A	492	43.363	-20.680	36.388	1.00	76.47	O
ATOM	3835	N	HIS	A	493	42.914	-20.119	34.253	1.00	74.04	N
ATOM	3836	CA	HIS	A	493	41.662	-19.477	34.596	1.00	71.39	C
ATOM	3837	CB	HIS	A	493	41.570	-18.100	33.949	1.00	74.23	C
ATOM	3838	CG	HIS	A	493	42.474	-17.079	34.566	1.00	76.40	C
ATOM	3839	CD2	HIS	A	493	43.460	-16.321	34.032	1.00	76.69	C
ATOM	3840	ND1	HIS	A	493	42.393	-16.719	35.892	1.00	78.14	N
ATOM	3841	CE1	HIS	A	493	43.289	-15.783	36.149	1.00	78.20	C
ATOM	3842	NE2	HIS	A	493	43.949	-15.524	35.037	1.00	75.53	N
ATOM	3843	C	HIS	A	493	40.462	-20.310	34.187	1.00	69.80	C
ATOM	3844	O	HIS	A	493	40.199	-20.520	33.009	1.00	69.35	O
ATOM	3845	N	ASP	A	494	39.745	-20.772	35.200	1.00	69.30	N
ATOM	3846	CA	ASP	A	494	38.534	-21.577	35.080	1.00	67.15	C
ATOM	3847	CB	ASP	A	494	38.227	-22.097	36.510	1.00	69.36	C
ATOM	3848	CG	ASP	A	494	36.746	-22.268	36.813	1.00	72.25	C
ATOM	3849	OD1	ASP	A	494	36.435	-22.520	37.998	1.00	72.88	O
ATOM	3850	OD2	ASP	A	494	35.893	-22.165	35.912	1.00	74.42	O
ATOM	3851	C	ASP	A	494	37.401	-20.727	34.466	1.00	62.95	C
ATOM	3852	O	ASP	A	494	37.483	-19.511	34.432	1.00	60.61	O
ATOM	3853	N	GLU	A	495	36.363	-21.366	33.948	1.00	62.76	N
ATOM	3854	CA	GLU	A	495	35.241	-20.638	33.364	1.00	66.35	C
ATOM	3855	CB	GLU	A	495	34.359	-21.593	32.554	1.00	71.34	C
ATOM	3856	CG	GLU	A	495	35.133	-22.508	31.601	1.00	76.37	C
ATOM	3857	CD	GLU	A	495	35.695	-21.787	30.387	1.00	77.38	C
ATOM	3858	OE1	GLU	A	495	36.517	-22.404	29.679	1.00	77.34	O
ATOM	3859	OE2	GLU	A	495	35.312	-20.619	30.134	1.00	79.15	O
ATOM	3860	C	GLU	A	495	34.413	-19.979	34.467	1.00	65.70	C
ATOM	3861	O	GLU	A	495	33.213	-19.775	34.344	1.00	64.12	O
ATOM	3862	N	THR	A	496	35.074	-19.663	35.564	1.00	69.16	N

359/396

Figure 3B-70

ATOM	3863	CA	THR	A	496	34.438	-19.010	36.698	1.00	71.50	C
ATOM	3864	CB	THR	A	496	35.006	-19.578	38.029	1.00	72.06	C
ATOM	3865	OG1	THR	A	496	34.256	-19.087	39.142	1.00	74.13	O
ATOM	3866	CG2	THR	A	496	36.451	-19.160	38.198	1.00	74.09	C
ATOM	3867	C	THR	A	496	34.836	-17.538	36.540	1.00	72.73	C
ATOM	3868	O	THR	A	496	34.144	-16.626	37.007	1.00	72.85	O
ATOM	3869	N	TYR	A	497	35.964	-17.339	35.853	1.00	72.19	N
ATOM	3870	CA	TYR	A	497	36.535	-16.024	35.581	1.00	70.67	C
ATOM	3871	CB	TYR	A	497	37.978	-16.169	35.129	1.00	69.06	C
ATOM	3872	CG	TYR	A	497	38.937	-16.482	36.240	1.00	70.91	C
ATOM	3873	CD1	TYR	A	497	39.672	-15.478	36.846	1.00	71.24	C
ATOM	3874	CE1	TYR	A	497	40.590	-15.767	37.837	1.00	70.83	C
ATOM	3875	CD2	TYR	A	497	39.138	-17.785	36.661	1.00	70.71	C
ATOM	3876	CE2	TYR	A	497	40.056	-18.081	37.650	1.00	71.34	C
ATOM	3877	CZ	TYR	A	497	40.782	-17.071	38.231	1.00	69.16	C
ATOM	3878	OH	TYR	A	497	41.728	-17.366	39.181	1.00	66.62	O
ATOM	3879	C	TYR	A	497	35.797	-15.223	34.527	1.00	70.43	C
ATOM	3880	O	TYR	A	497	34.627	-15.467	34.234	1.00	70.93	O
ATOM	3881	N	CYS	A	498	36.510	-14.254	33.964	1.00	68.57	N
ATOM	3882	CA	CYS	A	498	35.962	-13.392	32.937	1.00	67.29	C
ATOM	3883	CB	CYS	A	498	34.626	-12.820	33.372	1.00	65.90	C
ATOM	3884	SG	CYS	A	498	33.641	-12.419	31.949	1.00	75.24	S
ATOM	3885	C	CYS	A	498	36.940	-12.268	32.658	1.00	66.42	C
ATOM	3886	O	CYS	A	498	36.605	-11.092	32.704	1.00	64.69	O
ATOM	3887	N	ASP	A	499	38.166	-12.663	32.366	1.00	68.35	N
ATOM	3888	CA	ASP	A	499	39.239	-11.737	32.078	1.00	69.30	C
ATOM	3889	CB	ASP	A	499	40.475	-12.532	31.651	1.00	69.57	C
ATOM	3890	CG	ASP	A	499	41.021	-13.402	32.778	1.00	71.54	C
ATOM	3891	OD1	ASP	A	499	41.789	-14.339	32.485	1.00	68.64	O
ATOM	3892	OD2	ASP	A	499	40.687	-13.141	33.959	1.00	72.89	O
ATOM	3893	C	ASP	A	499	38.892	-10.680	31.037	1.00	68.51	C
ATOM	3894	O	ASP	A	499	39.240	-9.518	31.202	1.00	71.92	O
ATOM	3895	N	PRO	A	500	38.202	-11.055	29.953	1.00	66.28	N
ATOM	3896	CD	PRO	A	500	37.725	-12.363	29.476	1.00	69.40	C
ATOM	3897	CA	PRO	A	500	37.891	-10.009	28.982	1.00	65.64	C
ATOM	3898	CB	PRO	A	500	37.561	-10.801	27.722	1.00	65.59	C
ATOM	3899	CG	PRO	A	500	36.860	-11.982	28.271	1.00	67.80	C
ATOM	3900	C	PRO	A	500	36.735	-9.126	29.442	1.00	64.87	C
ATOM	3901	O	PRO	A	500	36.035	-8.535	28.623	1.00	67.11	O
ATOM	3902	N	ALA	A	501	36.536	-9.045	30.753	1.00	62.78	N
ATOM	3903	CA	ALA	A	501	35.475	-8.224	31.326	1.00	58.80	C
ATOM	3904	CB	ALA	A	501	34.356	-9.096	31.856	1.00	59.71	C
ATOM	3905	C	ALA	A	501	36.059	-7.405	32.452	1.00	55.76	C
ATOM	3906	O	ALA	A	501	35.353	-6.975	33.349	1.00	55.49	O
ATOM	3907	N	SER	A	502	37.365	-7.204	32.397	1.00	54.43	N
ATOM	3908	CA	SER	A	502	38.070	-6.441	33.409	1.00	53.87	C
ATOM	3909	CB	SER	A	502	38.941	-7.373	34.264	1.00	55.19	C
ATOM	3910	OG	SER	A	502	39.994	-7.954	33.510	1.00	55.59	O
ATOM	3911	C	SER	A	502	38.938	-5.409	32.704	1.00	53.78	C
ATOM	3912	O	SER	A	502	39.945	-4.949	33.240	1.00	51.32	O
ATOM	3913	N	LEU	A	503	38.540	-5.067	31.481	1.00	52.65	N
ATOM	3914	CA	LEU	A	503	39.256	-4.086	30.687	1.00	47.64	C
ATOM	3915	CB	LEU	A	503	39.755	-4.707	29.390	1.00	44.05	C
ATOM	3916	CG	LEU	A	503	40.709	-3.948	28.451	1.00	42.30	C
ATOM	3917	CD1	LEU	A	503	40.270	-4.205	27.011	1.00	44.25	C
ATOM	3918	CD2	LEU	A	503	40.723	-2.469	28.724	1.00	40.48	C

360/396

Figure 3B-71

ATOM	3919	C	LEU	A	503	38.295	-2.976	30.343	1.00	48.06	C
ATOM	3920	O	LEU	A	503	38.059	-2.734	29.170	1.00	53.99	O
ATOM	3921	N	PHE	A	504	37.731	-2.314	31.349	1.00	46.86	N
ATOM	3922	CA	PHE	A	504	36.803	-1.201	31.123	1.00	46.87	C
ATOM	3923	CB	PHE	A	504	37.572	0.115	31.000	1.00	44.20	C
ATOM	3924	CG	PHE	A	504	36.689	1.312	30.851	1.00	42.63	C
ATOM	3925	CD1	PHE	A	504	35.833	1.689	31.878	1.00	43.02	C
ATOM	3926	CD2	PHE	A	504	36.702	2.054	29.692	1.00	41.86	C
ATOM	3927	CE1	PHE	A	504	35.011	2.775	31.754	1.00	36.91	C
ATOM	3928	CE2	PHE	A	504	35.882	3.146	29.556	1.00	40.61	C
ATOM	3929	CZ	PHE	A	504	35.035	3.506	30.591	1.00	42.34	C
ATOM	3930	C	PHE	A	504	35.985	-1.410	29.857	1.00	47.91	C
ATOM	3931	O	PHE	A	504	34.932	-2.052	29.900	1.00	51.13	O
ATOM	3932	N	HIS	A	505	36.477	-0.849	28.747	1.00	43.88	N
ATOM	3933	CA	HIS	A	505	35.867	-0.972	27.427	1.00	40.38	C
ATOM	3934	CB	HIS	A	505	36.952	-1.238	26.408	1.00	39.56	C
ATOM	3935	CG	HIS	A	505	37.981	-0.165	26.363	1.00	40.33	C
ATOM	3936	CD2	HIS	A	505	38.956	0.161	27.239	1.00	35.22	C
ATOM	3937	ND1	HIS	A	505	38.005	0.798	25.378	1.00	39.74	N
ATOM	3938	CE1	HIS	A	505	38.949	1.677	25.654	1.00	36.36	C
ATOM	3939	NE2	HIS	A	505	39.539	1.313	26.778	1.00	39.41	N
ATOM	3940	C	HIS	A	505	34.864	-2.096	27.372	1.00	43.32	C
ATOM	3941	O	HIS	A	505	33.740	-1.913	26.957	1.00	45.14	O
ATOM	3942	N	VAL	A	506	35.273	-3.286	27.773	1.00	45.06	N
ATOM	3943	CA	VAL	A	506	34.338	-4.381	27.771	1.00	45.58	C
ATOM	3944	CB	VAL	A	506	35.015	-5.693	28.188	1.00	45.19	C
ATOM	3945	CG1	VAL	A	506	33.965	-6.786	28.337	1.00	42.51	C
ATOM	3946	CG2	VAL	A	506	36.064	-6.079	27.146	1.00	42.24	C
ATOM	3947	C	VAL	A	506	33.205	-4.042	28.738	1.00	46.94	C
ATOM	3948	O	VAL	A	506	32.174	-3.541	28.321	1.00	50.95	O
ATOM	3949	N	SER	A	507	33.409	-4.270	30.028	1.00	46.83	N
ATOM	3950	CA	SER	A	507	32.375	-4.011	31.032	1.00	47.39	C
ATOM	3951	CB	SER	A	507	32.983	-4.117	32.431	1.00	47.15	C
ATOM	3952	OG	SER	A	507	34.168	-3.351	32.524	1.00	52.38	O
ATOM	3953	C	SER	A	507	31.526	-2.734	30.951	1.00	47.05	C
ATOM	3954	O	SER	A	507	30.518	-2.640	31.650	1.00	47.74	O
ATOM	3955	N	ASN	A	508	31.904	-1.756	30.125	1.00	47.01	N
ATOM	3956	CA	ASN	A	508	31.119	-0.512	30.010	1.00	47.08	C
ATOM	3957	CB	ASN	A	508	31.925	0.709	30.478	1.00	49.78	C
ATOM	3958	CG	ASN	A	508	32.782	0.423	31.697	1.00	51.07	C
ATOM	3959	OD1	ASN	A	508	32.412	0.724	32.834	1.00	51.52	O
ATOM	3960	ND2	ASN	A	508	33.933	-0.175	31.459	1.00	50.59	N
ATOM	3961	C	ASN	A	508	30.747	-0.278	28.560	1.00	45.17	C
ATOM	3962	O	ASN	A	508	30.743	0.857	28.103	1.00	45.51	O
ATOM	3963	N	ASP	A	509	30.431	-1.354	27.851	1.00	43.54	N
ATOM	3964	CA	ASP	A	509	30.099	-1.300	26.437	1.00	41.53	C
ATOM	3965	CB	ASP	A	509	28.897	-0.421	26.193	1.00	48.22	C
ATOM	3966	CG	ASP	A	509	27.621	-1.149	26.464	1.00	55.23	C
ATOM	3967	OD1	ASP	A	509	27.525	-2.306	26.005	1.00	60.24	O
ATOM	3968	OD2	ASP	A	509	26.723	-0.584	27.125	1.00	60.80	O
ATOM	3969	C	ASP	A	509	31.269	-0.851	25.594	1.00	39.08	C
ATOM	3970	O	ASP	A	509	32.231	-1.579	25.474	1.00	42.91	O
ATOM	3971	N	TYR	A	510	31.210	0.324	24.994	1.00	35.55	N
ATOM	3972	CA	TYR	A	510	32.331	0.786	24.163	1.00	37.81	C
ATOM	3973	CB	TYR	A	510	33.447	1.374	25.055	1.00	36.41	C
ATOM	3974	CG	TYR	A	510	32.959	2.615	25.739	1.00	34.46	C

361/396

Figure 3B-72

ATOM	3975	CD1	TYR	A	510	32.592	3.713	24.997	1.00	32.78	C
ATOM	3976	CE1	TYR	A	510	31.910	4.745	25.547	1.00	33.37	C
ATOM	3977	CD2	TYR	A	510	32.644	2.608	27.074	1.00	35.86	C
ATOM	3978	CE2	TYR	A	510	31.954	3.645	27.640	1.00	38.29	C
ATOM	3979	CZ	TYR	A	510	31.581	4.713	26.866	1.00	37.02	C
ATOM	3980	OH	TYR	A	510	30.830	5.743	27.396	1.00	43.27	O
ATOM	3981	C	TYR	A	510	32.922	-0.251	23.204	1.00	36.83	C
ATOM	3982	O	TYR	A	510	33.633	-1.152	23.614	1.00	37.07	O
ATOM	3983	N	SER	A	511	32.617	-0.126	21.920	1.00	38.34	N
ATOM	3984	CA	SER	A	511	33.158	-1.049	20.937	1.00	39.82	C
ATOM	3985	CB	SER	A	511	32.717	-0.625	19.547	1.00	43.53	C
ATOM	3986	OG	SER	A	511	33.145	0.704	19.280	1.00	44.77	O
ATOM	3987	C	SER	A	511	34.673	-0.914	21.051	1.00	41.40	C
ATOM	3988	O	SER	A	511	35.169	0.135	21.468	1.00	42.38	O
ATOM	3989	N	PHE	A	512	35.424	-1.939	20.669	1.00	40.00	N
ATOM	3990	CA	PHE	A	512	36.866	-1.828	20.802	1.00	39.32	C
ATOM	3991	CB	PHE	A	512	37.398	-3.013	21.635	1.00	40.45	C
ATOM	3992	CG	PHE	A	512	38.667	-2.696	22.373	1.00	36.63	C
ATOM	3993	CD1	PHE	A	512	39.877	-3.205	21.943	1.00	31.13	C
ATOM	3994	CD2	PHE	A	512	38.660	-1.764	23.397	1.00	31.23	C
ATOM	3995	CE1	PHE	A	512	41.043	-2.781	22.502	1.00	33.53	C
ATOM	3996	CE2	PHE	A	512	39.829	-1.343	23.951	1.00	34.45	C
ATOM	3997	CZ	PHE	A	512	41.025	-1.848	23.502	1.00	32.97	C
ATOM	3998	C	PHE	A	512	37.645	-1.688	19.497	1.00	40.60	C
ATOM	3999	O	PHE	A	512	38.707	-1.059	19.458	1.00	39.95	O
ATOM	4000	N	ILE	A	513	37.099	-2.241	18.420	1.00	42.20	N
ATOM	4001	CA	ILE	A	513	37.752	-2.204	17.109	1.00	41.33	C
ATOM	4002	CB	ILE	A	513	36.905	-2.964	16.051	1.00	43.37	C
ATOM	4003	CG2	ILE	A	513	35.834	-2.048	15.509	1.00	43.79	C
ATOM	4004	CG1	ILE	A	513	37.804	-3.487	14.915	1.00	45.52	C
ATOM	4005	CD1	ILE	A	513	38.923	-4.431	15.370	1.00	43.35	C
ATOM	4006	C	ILE	A	513	38.086	-0.806	16.578	1.00	38.99	C
ATOM	4007	O	ILE	A	513	38.900	-0.676	15.666	1.00	38.16	O
ATOM	4008	N	ARG	A	514	37.477	0.236	17.134	1.00	38.05	N
ATOM	4009	CA	ARG	A	514	37.790	1.583	16.674	1.00	40.23	C
ATOM	4010	CB	ARG	A	514	36.908	2.639	17.345	1.00	40.51	C
ATOM	4011	CG	ARG	A	514	36.163	2.195	18.567	1.00	40.79	C
ATOM	4012	CD	ARG	A	514	36.760	2.837	19.775	1.00	44.27	C
ATOM	4013	NE	ARG	A	514	35.976	3.941	20.325	1.00	45.05	N
ATOM	4014	CZ	ARG	A	514	34.727	3.832	20.766	1.00	44.44	C
ATOM	4015	NH1	ARG	A	514	34.099	2.666	20.703	1.00	43.56	N
ATOM	4016	NH2	ARG	A	514	34.126	4.875	21.331	1.00	44.44	N
ATOM	4017	C	ARG	A	514	39.249	1.912	16.927	1.00	42.90	C
ATOM	4018	O	ARG	A	514	39.800	2.831	16.320	1.00	42.41	O
ATOM	4019	N	TYR	A	515	39.878	1.147	17.820	1.00	43.56	N
ATOM	4020	CA	TYR	A	515	41.282	1.352	18.149	1.00	39.44	C
ATOM	4021	CB	TYR	A	515	41.572	0.773	19.512	1.00	36.25	C
ATOM	4022	CG	TYR	A	515	40.790	1.471	20.592	1.00	33.29	C
ATOM	4023	CD1	TYR	A	515	41.004	2.808	20.884	1.00	26.76	C
ATOM	4024	CE1	TYR	A	515	40.257	3.452	21.850	1.00	24.53	C
ATOM	4025	CD2	TYR	A	515	39.812	0.801	21.297	1.00	36.67	C
ATOM	4026	CE2	TYR	A	515	39.067	1.437	22.266	1.00	36.62	C
ATOM	4027	CZ	TYR	A	515	39.296	2.757	22.538	1.00	28.75	C
ATOM	4028	OH	TYR	A	515	38.574	3.338	23.542	1.00	28.82	O
ATOM	4029	C	TYR	A	515	42.145	0.708	17.101	1.00	39.11	C
ATOM	4030	O	TYR	A	515	43.262	1.126	16.855	1.00	40.03	O

362/396

Figure 3B-73

ATOM	4031	N	TYR	A	516	41.612	-0.320	16.468	1.00	42.00	N
ATOM	4032	CA	TYR	A	516	42.338	-0.980	15.400	1.00	44.66	C
ATOM	4033	CB	TYR	A	516	41.655	-2.284	15.016	1.00	46.96	C
ATOM	4034	CG	TYR	A	516	42.374	-2.975	13.894	1.00	49.04	C
ATOM	4035	CD1	TYR	A	516	43.312	-3.959	14.150	1.00	47.92	C
ATOM	4036	CE1	TYR	A	516	44.027	-4.531	13.125	1.00	51.18	C
ATOM	4037	CD2	TYR	A	516	42.169	-2.587	12.577	1.00	48.37	C
ATOM	4038	CE2	TYR	A	516	42.881	-3.153	11.554	1.00	50.86	C
ATOM	4039	CZ	TYR	A	516	43.806	-4.120	11.832	1.00	51.40	C
ATOM	4040	OH	TYR	A	516	44.527	-4.666	10.807	1.00	56.52	O
ATOM	4041	C	TYR	A	516	42.317	-0.049	14.190	1.00	43.91	C
ATOM	4042	O	TYR	A	516	43.365	0.390	13.682	1.00	40.33	O
ATOM	4043	N	THR	A	517	41.092	0.225	13.738	1.00	43.68	N
ATOM	4044	CA	THR	A	517	40.802	1.103	12.594	1.00	38.64	C
ATOM	4045	CB	THR	A	517	39.336	1.284	12.477	1.00	37.18	C
ATOM	4046	OG1	THR	A	517	38.827	1.566	13.786	1.00	35.80	O
ATOM	4047	CG2	THR	A	517	38.694	0.017	11.932	1.00	32.94	C
ATOM	4048	C	THR	A	517	41.436	2.466	12.768	1.00	34.38	C
ATOM	4049	O	THR	A	517	41.997	3.023	11.837	1.00	26.93	O
ATOM	4050	N	ARG	A	518	41.332	3.002	13.973	1.00	34.58	N
ATOM	4051	CA	ARG	A	518	41.941	4.285	14.267	1.00	39.01	C
ATOM	4052	CB	ARG	A	518	41.701	4.670	15.710	1.00	40.18	C
ATOM	4053	CG	ARG	A	518	42.867	5.409	16.317	1.00	44.73	C
ATOM	4054	CD	ARG	A	518	43.498	4.609	17.444	1.00	50.25	C
ATOM	4055	NE	ARG	A	518	43.985	5.498	18.490	1.00	52.91	N
ATOM	4056	CZ	ARG	A	518	44.029	5.170	19.774	1.00	55.20	C
ATOM	4057	NH1	ARG	A	518	44.480	6.043	20.668	1.00	55.11	N
ATOM	4058	NH2	ARG	A	518	43.623	3.967	20.160	1.00	54.40	N
ATOM	4059	C	ARG	A	518	43.444	4.263	14.033	1.00	40.72	C
ATOM	4060	O	ARG	A	518	43.992	5.198	13.478	1.00	41.13	O
ATOM	4061	N	THR	A	519	44.110	3.193	14.464	1.00	45.37	N
ATOM	4062	CA	THR	A	519	45.562	3.081	14.325	1.00	45.19	C
ATOM	4063	CB	THR	A	519	46.092	1.763	14.931	1.00	46.01	C
ATOM	4064	OG1	THR	A	519	46.010	1.838	16.361	1.00	44.38	O
ATOM	4065	CG2	THR	A	519	47.542	1.515	14.513	1.00	41.77	C
ATOM	4066	C	THR	A	519	46.001	3.201	12.887	1.00	46.04	C
ATOM	4067	O	THR	A	519	47.004	3.867	12.604	1.00	44.51	O
ATOM	4068	N	LEU	A	520	45.251	2.567	11.981	1.00	46.71	N
ATOM	4069	CA	LEU	A	520	45.561	2.650	10.557	1.00	45.17	C
ATOM	4070	CB	LEU	A	520	44.884	1.543	9.772	1.00	46.89	C
ATOM	4071	CG	LEU	A	520	45.778	0.339	9.510	1.00	51.32	C
ATOM	4072	CD1	LEU	A	520	45.807	-0.533	10.741	1.00	54.19	C
ATOM	4073	CD2	LEU	A	520	45.261	-0.442	8.302	1.00	51.53	C
ATOM	4074	C	LEU	A	520	45.176	3.999	9.950	1.00	45.56	C
ATOM	4075	O	LEU	A	520	45.954	4.533	9.162	1.00	46.16	O
ATOM	4076	N	TYR	A	521	44.000	4.550	10.295	1.00	42.88	N
ATOM	4077	CA	TYR	A	521	43.613	5.860	9.754	1.00	42.05	C
ATOM	4078	CB	TYR	A	521	42.317	6.409	10.366	1.00	39.17	C
ATOM	4079	CG	TYR	A	521	41.049	5.670	10.028	1.00	37.54	C
ATOM	4080	CD1	TYR	A	521	40.913	4.994	8.824	1.00	35.54	C
ATOM	4081	CE1	TYR	A	521	39.770	4.256	8.545	1.00	37.75	C
ATOM	4082	CD2	TYR	A	521	40.001	5.606	10.949	1.00	36.68	C
ATOM	4083	CE2	TYR	A	521	38.862	4.876	10.688	1.00	38.20	C
ATOM	4084	CZ	TYR	A	521	38.753	4.199	9.482	1.00	41.51	C
ATOM	4085	OH	TYR	A	521	37.637	3.446	9.225	1.00	41.85	O
ATOM	4086	C	TYR	A	521	44.732	6.815	10.127	1.00	42.44	C

363/396

Figure 3B-74

ATOM	4087	O	TYR	A	521	45.279	7.528	9.299	1.00	44.44	O
ATOM	4088	N	GLN	A	522	45.046	6.811	11.407	1.00	44.38	N
ATOM	4089	CA	GLN	A	522	46.090	7.624	12.000	1.00	47.19	C
ATOM	4090	CB	GLN	A	522	46.630	6.870	13.213	1.00	51.15	C
ATOM	4091	CG	GLN	A	522	47.468	7.663	14.170	1.00	55.81	C
ATOM	4092	CD	GLN	A	522	48.242	6.755	15.108	1.00	58.62	C
ATOM	4093	OE1	GLN	A	522	47.669	5.910	15.806	1.00	55.40	O
ATOM	4094	NE2	GLN	A	522	49.557	6.923	15.124	1.00	60.37	N
ATOM	4095	C	GLN	A	522	47.245	7.979	11.060	1.00	46.70	C
ATOM	4096	O	GLN	A	522	47.577	9.153	10.894	1.00	46.67	O
ATOM	4097	N	PHE	A	523	47.861	6.973	10.444	1.00	45.18	N
ATOM	4098	CA	PHE	A	523	49.004	7.227	9.561	1.00	45.46	C
ATOM	4099	CB	PHE	A	523	49.909	5.998	9.520	1.00	42.75	C
ATOM	4100	CG	PHE	A	523	50.468	5.660	10.840	1.00	41.74	C
ATOM	4101	CD1	PHE	A	523	51.400	6.496	11.433	1.00	42.00	C
ATOM	4102	CD2	PHE	A	523	49.979	4.585	11.549	1.00	41.63	C
ATOM	4103	CE1	PHE	A	523	51.824	6.270	12.715	1.00	45.07	C
ATOM	4104	CE2	PHE	A	523	50.398	4.348	12.841	1.00	46.55	C
ATOM	4105	CZ	PHE	A	523	51.321	5.192	13.428	1.00	45.82	C
ATOM	4106	C	PHE	A	523	48.690	7.683	8.151	1.00	45.74	C
ATOM	4107	O	PHE	A	523	49.562	8.193	7.463	1.00	45.11	O
ATOM	4108	N	GLN	A	524	47.448	7.483	7.721	1.00	47.36	N
ATOM	4109	CA	GLN	A	524	47.019	7.901	6.400	1.00	44.16	C
ATOM	4110	CB	GLN	A	524	45.685	7.268	6.053	1.00	39.19	C
ATOM	4111	CG	GLN	A	524	45.681	5.777	6.206	1.00	36.20	C
ATOM	4112	CD	GLN	A	524	44.601	5.111	5.395	1.00	33.45	C
ATOM	4113	OE1	GLN	A	524	44.598	5.201	4.167	1.00	33.70	O
ATOM	4114	NE2	GLN	A	524	43.681	4.433	6.070	1.00	26.15	N
ATOM	4115	C	GLN	A	524	46.869	9.399	6.486	1.00	46.57	C
ATOM	4116	O	GLN	A	524	47.348	10.128	5.624	1.00	46.62	O
ATOM	4117	N	PHE	A	525	46.210	9.852	7.547	1.00	49.37	N
ATOM	4118	CA	PHE	A	525	46.002	11.277	7.768	1.00	56.55	C
ATOM	4119	CB	PHE	A	525	45.111	11.508	8.993	1.00	58.06	C
ATOM	4120	CG	PHE	A	525	43.694	11.061	8.813	1.00	60.65	C
ATOM	4121	CD1	PHE	A	525	43.359	9.729	8.883	1.00	59.78	C
ATOM	4122	CD2	PHE	A	525	42.694	11.985	8.579	1.00	63.76	C
ATOM	4123	CE1	PHE	A	525	42.056	9.325	8.727	1.00	61.45	C
ATOM	4124	CE2	PHE	A	525	41.385	11.584	8.420	1.00	64.88	C
ATOM	4125	CZ	PHE	A	525	41.068	10.251	8.496	1.00	63.45	C
ATOM	4126	C	PHE	A	525	47.324	12.012	7.987	1.00	59.07	C
ATOM	4127	O	PHE	A	525	47.463	13.202	7.680	1.00	56.23	O
ATOM	4128	N	GLN	A	526	48.300	11.302	8.529	1.00	62.69	N
ATOM	4129	CA	GLN	A	526	49.565	11.936	8.796	1.00	66.35	C
ATOM	4130	CB	GLN	A	526	50.322	11.166	9.872	1.00	67.04	C
ATOM	4131	CG	GLN	A	526	51.512	11.928	10.441	1.00	70.28	C
ATOM	4132	CD	GLN	A	526	51.111	13.108	11.319	1.00	69.82	C
ATOM	4133	OE1	GLN	A	526	51.954	13.927	11.692	1.00	68.06	O
ATOM	4134	NE2	GLN	A	526	49.827	13.191	11.663	1.00	68.44	N
ATOM	4135	C	GLN	A	526	50.400	12.053	7.534	1.00	68.78	C
ATOM	4136	O	GLN	A	526	51.094	13.044	7.353	1.00	72.53	O
ATOM	4137	N	GLU	A	527	50.324	11.065	6.648	1.00	68.61	N
ATOM	4138	CA	GLU	A	527	51.109	11.115	5.418	1.00	68.44	C
ATOM	4139	CB	GLU	A	527	51.131	9.761	4.716	1.00	70.62	C
ATOM	4140	CG	GLU	A	527	52.288	9.599	3.744	1.00	78.64	C
ATOM	4141	CD	GLU	A	527	52.339	8.212	3.109	1.00	85.89	C
ATOM	4142	OE1	GLU	A	527	51.537	7.951	2.181	1.00	87.78	O

364/396

Figure 3B-75

ATOM	4143	OE2	GLU	A	527	53.175	7.381	3.543	1.00	86.40	O
ATOM	4144	C	GLU	A	527	50.526	12.137	4.473	1.00	68.39	C
ATOM	4145	O	GLU	A	527	51.090	12.393	3.411	1.00	72.52	O
ATOM	4146	N	ALA	A	528	49.395	12.718	4.865	1.00	65.67	N
ATOM	4147	CA	ALA	A	528	48.712	13.715	4.053	1.00	61.57	C
ATOM	4148	CB	ALA	A	528	47.222	13.489	4.104	1.00	58.59	C
ATOM	4149	C	ALA	A	528	49.033	15.112	4.537	1.00	60.17	C
ATOM	4150	O	ALA	A	528	49.464	15.951	3.762	1.00	62.37	O
ATOM	4151	N	LEU	A	529	48.822	15.348	5.826	1.00	59.80	N
ATOM	4152	CA	LEU	A	529	49.071	16.643	6.455	1.00	61.49	C
ATOM	4153	CB	LEU	A	529	48.578	16.585	7.894	1.00	58.33	C
ATOM	4154	CG	LEU	A	529	47.184	15.990	8.052	1.00	53.66	C
ATOM	4155	CD1	LEU	A	529	46.970	15.590	9.476	1.00	52.81	C
ATOM	4156	CD2	LEU	A	529	46.148	16.986	7.615	1.00	51.90	C
ATOM	4157	C	LEU	A	529	50.550	17.080	6.427	1.00	64.75	C
ATOM	4158	O	LEU	A	529	50.860	18.261	6.266	1.00	61.27	O
ATOM	4159	N	CYS	A	530	51.466	16.135	6.605	1.00	69.91	N
ATOM	4160	CA	CYS	A	530	52.882	16.472	6.558	1.00	76.14	C
ATOM	4161	C	CYS	A	530	53.085	17.051	5.184	1.00	76.97	C
ATOM	4162	O	CYS	A	530	53.514	18.192	5.032	1.00	78.66	O
ATOM	4163	CB	CYS	A	530	53.747	15.222	6.739	1.00	80.25	C
ATOM	4164	SG	CYS	A	530	53.350	14.398	8.310	1.00	91.04	S
ATOM	4165	N	GLN	A	531	52.742	16.256	4.182	1.00	77.19	N
ATOM	4166	CA	GLN	A	531	52.854	16.687	2.803	1.00	77.55	C
ATOM	4167	CB	GLN	A	531	52.487	15.532	1.878	1.00	81.27	C
ATOM	4168	CG	GLN	A	531	53.069	15.654	0.489	1.00	86.76	C
ATOM	4169	CD	GLN	A	531	52.776	14.436	-0.345	1.00	89.31	C
ATOM	4170	OE1	GLN	A	531	53.221	14.332	-1.483	1.00	92.33	O
ATOM	4171	NE2	GLN	A	531	52.018	13.502	0.219	1.00	89.51	N
ATOM	4172	C	GLN	A	531	51.921	17.878	2.556	1.00	75.05	C
ATOM	4173	O	GLN	A	531	51.941	18.480	1.485	1.00	75.69	O
ATOM	4174	N	ALA	A	532	51.109	18.208	3.557	1.00	71.82	N
ATOM	4175	CA	ALA	A	532	50.175	19.324	3.471	1.00	68.95	C
ATOM	4176	CB	ALA	A	532	48.784	18.880	3.857	1.00	70.05	C
ATOM	4177	C	ALA	A	532	50.646	20.403	4.417	1.00	68.47	C
ATOM	4178	O	ALA	A	532	49.861	21.217	4.897	1.00	68.43	O
ATOM	4179	N	ALA	A	533	51.940	20.379	4.698	1.00	67.65	N
ATOM	4180	CA	ALA	A	533	52.576	21.348	5.577	1.00	67.87	C
ATOM	4181	CB	ALA	A	533	52.515	20.881	7.017	1.00	68.12	C
ATOM	4182	C	ALA	A	533	54.008	21.372	5.097	1.00	67.98	C
ATOM	4183	O	ALA	A	533	54.905	21.881	5.765	1.00	67.85	O
ATOM	4184	N	LYS	A	534	54.196	20.789	3.920	1.00	67.78	N
ATOM	4185	CA	LYS	A	534	55.493	20.692	3.277	1.00	70.45	C
ATOM	4186	CB	LYS	A	534	55.933	22.072	2.764	1.00	71.48	C
ATOM	4187	CG	LYS	A	534	57.150	22.051	1.834	1.00	73.45	C
ATOM	4188	CD	LYS	A	534	56.882	21.221	0.590	1.00	75.84	C
ATOM	4189	CE	LYS	A	534	58.102	21.123	-0.311	1.00	77.95	C
ATOM	4190	NZ	LYS	A	534	57.855	20.158	-1.425	1.00	77.44	N
ATOM	4191	C	LYS	A	534	56.541	20.101	4.218	1.00	70.60	C
ATOM	4192	O	LYS	A	534	57.204	20.823	4.954	1.00	72.60	O
ATOM	4193	N	HIS	A	535	56.665	18.776	4.192	1.00	70.35	N
ATOM	4194	CA	HIS	A	535	57.626	18.050	5.013	1.00	69.13	C
ATOM	4195	CB	HIS	A	535	56.897	17.038	5.895	1.00	71.06	C
ATOM	4196	CG	HIS	A	535	57.809	16.097	6.619	1.00	74.19	C
ATOM	4197	CD2	HIS	A	535	57.971	14.756	6.514	1.00	73.95	C
ATOM	4198	ND1	HIS	A	535	58.707	16.517	7.577	1.00	76.41	N

365/396

Figure 3B-76

ATOM	4199	CE1	HIS	A	535	59.383	15.476	8.029	1.00	75.86	C
ATOM	4200	NE2	HIS	A	535	58.957	14.396	7.400	1.00	74.92	N
ATOM	4201	C	HIS	A	535	58.541	17.328	4.047	1.00	69.84	C
ATOM	4202	O	HIS	A	535	58.131	17.009	2.937	1.00	70.75	O
ATOM	4203	N	GLU	A	536	59.776	17.064	4.448	1.00	71.44	N
ATOM	4204	CA	GLU	A	536	60.697	16.377	3.547	1.00	74.86	C
ATOM	4205	CB	GLU	A	536	61.614	17.376	2.832	1.00	78.23	C
ATOM	4206	CG	GLU	A	536	61.588	17.292	1.312	1.00	78.69	C
ATOM	4207	CD	GLU	A	536	60.468	18.113	0.715	1.00	82.72	C
ATOM	4208	OE1	GLU	A	536	60.543	19.361	0.791	1.00	82.80	O
ATOM	4209	OE2	GLU	A	536	59.512	17.513	0.177	1.00	85.70	O
ATOM	4210	C	GLU	A	536	61.558	15.360	4.262	1.00	75.00	C
ATOM	4211	O	GLU	A	536	62.787	15.409	4.198	1.00	76.22	O
ATOM	4212	N	GLY	A	537	60.913	14.434	4.944	1.00	74.71	N
ATOM	4213	CA	GLY	A	537	61.652	13.411	5.648	1.00	76.49	C
ATOM	4214	C	GLY	A	537	60.665	12.310	5.908	1.00	76.54	C
ATOM	4215	O	GLY	A	537	59.523	12.406	5.464	1.00	79.04	O
ATOM	4216	N	PRO	A	538	61.067	11.236	6.585	1.00	75.29	N
ATOM	4217	CD	PRO	A	538	62.414	10.775	6.949	1.00	76.20	C
ATOM	4218	CA	PRO	A	538	60.071	10.194	6.825	1.00	75.04	C
ATOM	4219	CB	PRO	A	538	60.874	9.120	7.547	1.00	76.39	C
ATOM	4220	CG	PRO	A	538	62.239	9.269	6.940	1.00	75.87	C
ATOM	4221	C	PRO	A	538	59.010	10.839	7.707	1.00	73.31	C
ATOM	4222	O	PRO	A	538	59.304	11.802	8.420	1.00	72.38	O
ATOM	4223	N	LEU	A	539	57.783	10.339	7.664	1.00	70.50	N
ATOM	4224	CA	LEU	A	539	56.747	10.954	8.478	1.00	70.64	C
ATOM	4225	CB	LEU	A	539	55.354	10.415	8.110	1.00	67.03	C
ATOM	4226	CG	LEU	A	539	55.079	8.926	7.956	1.00	61.96	C
ATOM	4227	CD1	LEU	A	539	53.596	8.737	7.839	1.00	59.90	C
ATOM	4228	CD2	LEU	A	539	55.801	8.372	6.742	1.00	60.77	C
ATOM	4229	C	LEU	A	539	56.983	10.826	9.973	1.00	72.10	C
ATOM	4230	O	LEU	A	539	56.335	11.523	10.759	1.00	71.68	O
ATOM	4231	N	HIS	A	540	57.910	9.944	10.358	1.00	75.32	N
ATOM	4232	CA	HIS	A	540	58.249	9.727	11.765	1.00	77.40	C
ATOM	4233	CB	HIS	A	540	58.825	8.318	11.981	1.00	80.83	C
ATOM	4234	CG	HIS	A	540	60.217	8.125	11.450	1.00	86.74	C
ATOM	4235	CD2	HIS	A	540	61.102	8.995	10.906	1.00	89.09	C
ATOM	4236	ND1	HIS	A	540	60.852	6.901	11.470	1.00	88.65	N
ATOM	4237	CE1	HIS	A	540	62.067	7.026	10.964	1.00	88.92	C
ATOM	4238	NE2	HIS	A	540	62.244	8.286	10.615	1.00	90.63	N
ATOM	4239	C	HIS	A	540	59.259	10.784	12.186	1.00	78.12	C
ATOM	4240	O	HIS	A	540	60.041	10.600	13.106	1.00	80.84	O
ATOM	4241	N	LYS	A	541	59.235	11.896	11.473	1.00	78.09	N
ATOM	4242	CA	LYS	A	541	60.112	13.016	11.732	1.00	77.96	C
ATOM	4243	CB	LYS	A	541	61.294	12.989	10.769	1.00	81.01	C
ATOM	4244	CG	LYS	A	541	62.403	12.034	11.141	1.00	82.90	C
ATOM	4245	CD	LYS	A	541	63.201	12.584	12.296	1.00	83.92	C
ATOM	4246	CE	LYS	A	541	64.524	11.878	12.412	1.00	84.76	C
ATOM	4247	NZ	LYS	A	541	65.324	12.399	13.557	1.00	87.79	N
ATOM	4248	C	LYS	A	541	59.235	14.197	11.412	1.00	77.82	C
ATOM	4249	O	LYS	A	541	59.660	15.347	11.440	1.00	77.50	O
ATOM	4250	N	CYS	A	542	57.988	13.891	11.100	1.00	78.93	N
ATOM	4251	CA	CYS	A	542	57.038	14.914	10.737	1.00	81.80	C
ATOM	4252	C	CYS	A	542	56.466	15.693	11.908	1.00	81.02	C
ATOM	4253	O	CYS	A	542	55.863	15.132	12.824	1.00	79.82	O
ATOM	4254	CB	CYS	A	542	55.919	14.296	9.906	1.00	85.00	C

366/396

Figure 3B-77

ATOM	4255	SG	CYS	A	542	54.471	15.370	9.698	1.00	88.91	S
ATOM	4256	N	ASP	A	543	56.681	17.003	11.848	1.00	81.73	N
ATOM	4257	CA	ASP	A	543	56.218	17.957	12.843	1.00	81.37	C
ATOM	4258	CB	ASP	A	543	56.929	19.306	12.656	1.00	85.70	C
ATOM	4259	CG	ASP	A	543	57.660	19.434	11.299	1.00	89.14	C
ATOM	4260	OD1	ASP	A	543	58.210	20.528	11.041	1.00	90.47	O
ATOM	4261	OD2	ASP	A	543	57.705	18.473	10.492	1.00	88.77	O
ATOM	4262	C	ASP	A	543	54.714	18.132	12.697	1.00	80.11	C
ATOM	4263	O	ASP	A	543	53.962	17.311	13.203	1.00	81.06	O
ATOM	4264	N	ILE	A	544	54.297	19.193	11.999	1.00	77.58	N
ATOM	4265	CA	ILE	A	544	52.886	19.532	11.720	1.00	75.56	C
ATOM	4266	CB	ILE	A	544	51.918	18.334	11.934	1.00	74.11	C
ATOM	4267	CG2	ILE	A	544	51.421	18.315	13.380	1.00	77.50	C
ATOM	4268	CG1	ILE	A	544	50.659	18.503	11.089	1.00	71.95	C
ATOM	4269	CD1	ILE	A	544	49.474	19.052	11.871	1.00	67.68	C
ATOM	4270	C	ILE	A	544	52.391	20.680	12.586	1.00	75.57	C
ATOM	4271	O	ILE	A	544	51.286	21.186	12.394	1.00	72.63	O
ATOM	4272	N	SER	A	545	53.218	21.095	13.538	1.00	77.49	N
ATOM	4273	CA	SER	A	545	52.848	22.173	14.442	1.00	78.22	C
ATOM	4274	CB	SER	A	545	53.718	22.096	15.706	1.00	77.61	C
ATOM	4275	OG	SER	A	545	52.937	22.267	16.882	1.00	76.22	O
ATOM	4276	C	SER	A	545	52.979	23.546	13.759	1.00	78.50	C
ATOM	4277	O	SER	A	545	53.851	23.739	12.911	1.00	77.40	O
ATOM	4278	N	ASN	A	546	52.090	24.478	14.122	1.00	78.93	N
ATOM	4279	CA	ASN	A	546	52.071	25.845	13.579	1.00	78.87	C
ATOM	4280	CB	ASN	A	546	53.467	26.475	13.672	1.00	77.60	C
ATOM	4281	CG	ASN	A	546	53.841	26.849	15.089	1.00	74.52	C
ATOM	4282	OD1	ASN	A	546	54.992	26.697	15.500	1.00	73.31	O
ATOM	4283	ND2	ASN	A	546	52.868	27.353	15.843	1.00	72.22	N
ATOM	4284	C	ASN	A	546	51.560	25.954	12.143	1.00	79.38	C
ATOM	4285	O	ASN	A	546	51.401	27.060	11.614	1.00	79.60	O
ATOM	4286	N	SER	A	547	51.298	24.807	11.522	1.00	79.39	N
ATOM	4287	CA	SER	A	547	50.810	24.750	10.145	1.00	78.64	C
ATOM	4288	CB	SER	A	547	51.310	23.475	9.462	1.00	79.01	C
ATOM	4289	OG	SER	A	547	50.545	23.180	8.306	1.00	78.74	O
ATOM	4290	C	SER	A	547	49.296	24.779	10.055	1.00	77.47	C
ATOM	4291	O	SER	A	547	48.640	23.833	10.490	1.00	77.44	O
ATOM	4292	N	THR	A	548	48.742	25.857	9.500	1.00	75.23	N
ATOM	4293	CA	THR	A	548	47.293	25.952	9.341	1.00	73.92	C
ATOM	4294	CB	THR	A	548	46.823	27.399	9.253	1.00	70.90	C
ATOM	4295	OG1	THR	A	548	47.668	28.115	8.348	1.00	71.92	O
ATOM	4296	CG2	THR	A	548	46.862	28.046	10.619	1.00	68.67	C
ATOM	4297	C	THR	A	548	46.976	25.227	8.044	1.00	74.62	C
ATOM	4298	O	THR	A	548	45.847	24.788	7.802	1.00	72.17	O
ATOM	4299	N	GLU	A	549	48.005	25.097	7.217	1.00	74.88	N
ATOM	4300	CA	GLU	A	549	47.879	24.394	5.960	1.00	76.47	C
ATOM	4301	CB	GLU	A	549	49.253	24.275	5.300	1.00	78.90	C
ATOM	4302	CG	GLU	A	549	49.959	25.611	5.186	1.00	84.53	C
ATOM	4303	CD	GLU	A	549	48.992	26.723	4.817	1.00	88.92	C
ATOM	4304	OE1	GLU	A	549	48.326	26.598	3.768	1.00	93.68	O
ATOM	4305	OE2	GLU	A	549	48.887	27.717	5.571	1.00	89.95	O
ATOM	4306	C	GLU	A	549	47.349	23.025	6.347	1.00	75.74	C
ATOM	4307	O	GLU	A	549	46.515	22.442	5.654	1.00	78.18	O
ATOM	4308	N	ALA	A	550	47.834	22.539	7.486	1.00	73.37	N
ATOM	4309	CA	ALA	A	550	47.441	21.245	8.031	1.00	70.25	C
ATOM	4310	CB	ALA	A	550	48.588	20.660	8.855	1.00	67.96	C

367/396

Figure 3B-78

ATOM	4311	C	ALA	A	550	46.190	21.386	8.897	1.00	66.97	C
ATOM	4312	O	ALA	A	550	45.196	20.694	8.699	1.00	64.91	O
ATOM	4313	N	GLY	A	551	46.243	22.279	9.870	1.00	65.99	N
ATOM	4314	CA	GLY	A	551	45.085	22.462	10.711	1.00	66.68	C
ATOM	4315	C	GLY	A	551	43.866	22.678	9.842	1.00	68.14	C
ATOM	4316	O	GLY	A	551	42.871	21.949	9.950	1.00	64.97	O
ATOM	4317	N	GLN	A	552	43.962	23.670	8.955	1.00	69.94	N
ATOM	4318	CA	GLN	A	552	42.864	24.018	8.056	1.00	71.14	C
ATOM	4319	CB	GLN	A	552	43.302	25.091	7.052	1.00	72.41	C
ATOM	4320	CG	GLN	A	552	42.165	25.637	6.178	1.00	76.09	C
ATOM	4321	CD	GLN	A	552	40.995	26.219	6.977	1.00	77.15	C
ATOM	4322	OE1	GLN	A	552	41.140	27.215	7.704	1.00	76.59	O
ATOM	4323	NE2	GLN	A	552	39.826	25.598	6.836	1.00	74.61	N
ATOM	4324	C	GLN	A	552	42.330	22.805	7.315	1.00	69.12	C
ATOM	4325	O	GLN	A	552	41.127	22.555	7.319	1.00	68.48	O
ATOM	4326	N	LYS	A	553	43.220	22.051	6.679	1.00	66.93	N
ATOM	4327	CA	LYS	A	553	42.787	20.866	5.963	1.00	63.60	C
ATOM	4328	CB	LYS	A	553	43.994	20.045	5.486	1.00	58.07	C
ATOM	4329	CG	LYS	A	553	43.611	18.892	4.585	1.00	56.18	C
ATOM	4330	CD	LYS	A	553	44.797	18.273	3.871	1.00	60.10	C
ATOM	4331	CE	LYS	A	553	44.356	17.055	3.030	1.00	64.87	C
ATOM	4332	NZ	LYS	A	553	45.446	16.416	2.210	1.00	64.15	N
ATOM	4333	C	LYS	A	553	41.895	20.038	6.891	1.00	63.86	C
ATOM	4334	O	LYS	A	553	40.668	20.078	6.781	1.00	64.51	O
ATOM	4335	N	LEU	A	554	42.502	19.313	7.822	1.00	63.08	N
ATOM	4336	CA	LEU	A	554	41.742	18.479	8.749	1.00	62.93	C
ATOM	4337	CB	LEU	A	554	42.607	18.084	9.945	1.00	61.24	C
ATOM	4338	CG	LEU	A	554	41.946	17.193	10.996	1.00	53.38	C
ATOM	4339	CD1	LEU	A	554	41.971	15.764	10.537	1.00	48.67	C
ATOM	4340	CD2	LEU	A	554	42.675	17.338	12.304	1.00	51.48	C
ATOM	4341	C	LEU	A	554	40.473	19.145	9.266	1.00	64.67	C
ATOM	4342	O	LEU	A	554	39.496	18.465	9.575	1.00	63.25	O
ATOM	4343	N	PHE	A	555	40.483	20.470	9.377	1.00	67.23	N
ATOM	4344	CA	PHE	A	555	39.299	21.169	9.872	1.00	68.85	C
ATOM	4345	CB	PHE	A	555	39.531	22.678	9.965	1.00	71.43	C
ATOM	4346	CG	PHE	A	555	38.477	23.388	10.761	1.00	73.64	C
ATOM	4347	CD1	PHE	A	555	37.135	23.122	10.544	1.00	72.12	C
ATOM	4348	CD2	PHE	A	555	38.826	24.262	11.771	1.00	76.85	C
ATOM	4349	CE1	PHE	A	555	36.165	23.700	11.315	1.00	72.80	C
ATOM	4350	CE2	PHE	A	555	37.854	24.849	12.552	1.00	78.70	C
ATOM	4351	CZ	PHE	A	555	36.519	24.563	12.323	1.00	76.86	C
ATOM	4352	C	PHE	A	555	38.118	20.933	8.947	1.00	67.25	C
ATOM	4353	O	PHE	A	555	37.040	20.513	9.380	1.00	65.50	O
ATOM	4354	N	ASN	A	556	38.346	21.237	7.673	1.00	66.00	N
ATOM	4355	CA	ASN	A	556	37.356	21.093	6.619	1.00	65.43	C
ATOM	4356	CB	ASN	A	556	38.002	21.433	5.274	1.00	64.74	C
ATOM	4357	CG	ASN	A	556	38.681	22.795	5.283	1.00	65.05	C
ATOM	4358	OD1	ASN	A	556	39.625	23.037	4.533	1.00	65.44	O
ATOM	4359	ND2	ASN	A	556	38.197	23.691	6.130	1.00	63.97	N
ATOM	4360	C	ASN	A	556	36.832	19.667	6.605	1.00	65.63	C
ATOM	4361	O	ASN	A	556	35.839	19.370	5.946	1.00	65.23	O
ATOM	4362	N	MET	A	557	37.516	18.799	7.349	1.00	66.66	N
ATOM	4363	CA	MET	A	557	37.180	17.380	7.474	1.00	65.71	C
ATOM	4364	CB	MET	A	557	38.466	16.561	7.617	1.00	67.35	C
ATOM	4365	CG	MET	A	557	38.292	15.234	8.337	1.00	72.12	C
ATOM	4366	SD	MET	A	557	37.178	14.116	7.477	1.00	81.00	S

368/396

Figure 3B-79

ATOM	4367	CE	MET	A	557	35.831	13.936	8.698	1.00	80.15	C
ATOM	4368	C	MET	A	557	36.289	17.106	8.675	1.00	63.56	C
ATOM	4369	O	MET	A	557	35.207	16.536	8.554	1.00	60.71	O
ATOM	4370	N	LEU	A	558	36.777	17.515	9.837	1.00	64.75	N
ATOM	4371	CA	LEU	A	558	36.078	17.323	11.095	1.00	66.45	C
ATOM	4372	CB	LEU	A	558	36.859	17.994	12.225	1.00	68.05	C
ATOM	4373	CG	LEU	A	558	38.041	17.281	12.874	1.00	68.59	C
ATOM	4374	CD1	LEU	A	558	38.931	16.689	11.816	1.00	72.55	C
ATOM	4375	CD2	LEU	A	558	38.804	18.268	13.742	1.00	69.26	C
ATOM	4376	C	LEU	A	558	34.664	17.875	11.090	1.00	67.55	C
ATOM	4377	O	LEU	A	558	33.718	17.206	11.514	1.00	67.43	O
ATOM	4378	N	ARG	A	559	34.528	19.105	10.608	1.00	68.38	N
ATOM	4379	CA	ARG	A	559	33.240	19.775	10.590	1.00	67.35	C
ATOM	4380	CB	ARG	A	559	33.392	21.174	9.994	1.00	70.14	C
ATOM	4381	CG	ARG	A	559	34.147	21.218	8.692	1.00	80.31	C
ATOM	4382	CD	ARG	A	559	33.359	20.575	7.564	1.00	87.30	C
ATOM	4383	NE	ARG	A	559	33.179	21.490	6.437	1.00	93.78	N
ATOM	4384	CZ	ARG	A	559	32.486	22.625	6.497	1.00	95.50	C
ATOM	4385	NH1	ARG	A	559	31.899	22.994	7.632	1.00	93.43	N
ATOM	4386	NH2	ARG	A	559	32.381	23.395	5.419	1.00	96.68	N
ATOM	4387	C	ARG	A	559	32.076	19.051	9.934	1.00	64.62	C
ATOM	4388	O	ARG	A	559	30.938	19.288	10.319	1.00	68.75	O
ATOM	4389	N	LEU	A	560	32.330	18.167	8.972	1.00	58.21	N
ATOM	4390	CA	LEU	A	560	31.229	17.464	8.322	1.00	56.01	C
ATOM	4391	CB	LEU	A	560	31.707	16.698	7.083	1.00	58.16	C
ATOM	4392	CG	LEU	A	560	32.369	17.347	5.859	1.00	61.54	C
ATOM	4393	CD1	LEU	A	560	31.638	18.601	5.414	1.00	61.56	C
ATOM	4394	CD2	LEU	A	560	33.791	17.670	6.206	1.00	66.74	C
ATOM	4395	C	LEU	A	560	30.442	16.483	9.206	1.00	56.60	C
ATOM	4396	O	LEU	A	560	29.429	15.951	8.759	1.00	57.27	O
ATOM	4397	N	GLY	A	561	30.888	16.233	10.440	1.00	55.14	N
ATOM	4398	CA	GLY	A	561	30.179	15.298	11.307	1.00	50.64	C
ATOM	4399	C	GLY	A	561	30.131	13.926	10.660	1.00	50.99	C
ATOM	4400	O	GLY	A	561	31.133	13.475	10.120	1.00	50.07	O
ATOM	4401	N	LYS	A	562	28.982	13.259	10.714	1.00	53.61	N
ATOM	4402	CA	LYS	A	562	28.807	11.941	10.091	1.00	57.97	C
ATOM	4403	CB	LYS	A	562	28.294	10.915	11.103	1.00	58.23	C
ATOM	4404	CG	LYS	A	562	28.428	9.458	10.638	1.00	58.58	C
ATOM	4405	CD	LYS	A	562	28.505	8.521	11.839	1.00	59.51	C
ATOM	4406	CE	LYS	A	562	29.148	7.186	11.513	1.00	56.50	C
ATOM	4407	NZ	LYS	A	562	29.366	6.395	12.758	1.00	58.66	N
ATOM	4408	C	LYS	A	562	27.794	12.069	8.956	1.00	61.06	C
ATOM	4409	O	LYS	A	562	26.981	11.174	8.711	1.00	61.17	O
ATOM	4410	N	SER	A	563	27.861	13.200	8.269	1.00	61.43	N
ATOM	4411	CA	SER	A	563	26.967	13.493	7.171	1.00	63.07	C
ATOM	4412	CB	SER	A	563	26.623	14.976	7.184	1.00	64.65	C
ATOM	4413	OG	SER	A	563	27.783	15.744	6.914	1.00	67.15	O
ATOM	4414	C	SER	A	563	27.615	13.147	5.843	1.00	63.47	C
ATOM	4415	O	SER	A	563	27.307	13.753	4.824	1.00	64.15	O
ATOM	4416	N	GLU	A	564	28.520	12.181	5.851	1.00	64.10	N
ATOM	4417	CA	GLU	A	564	29.209	11.783	4.627	1.00	64.84	C
ATOM	4418	CB	GLU	A	564	30.254	12.820	4.235	1.00	63.21	C
ATOM	4419	CG	GLU	A	564	29.867	13.707	3.082	1.00	66.92	C
ATOM	4420	CD	GLU	A	564	31.037	14.547	2.588	1.00	70.29	C
ATOM	4421	OE1	GLU	A	564	32.086	13.976	2.227	1.00	70.60	O
ATOM	4422	OE2	GLU	A	564	30.915	15.784	2.557	1.00	74.23	O

369/396

Figure 3B-80

ATOM	4423	C	GLU	A	564	29.909	10.470	4.882	1.00	65.72	C
ATOM	4424	O	GLU	A	564	30.700	10.361	5.813	1.00	68.24	O
ATOM	4425	N	PRO	A	565	29.633	9.453	4.057	1.00	64.78	N
ATOM	4426	CD	PRO	A	565	28.802	9.456	2.842	1.00	63.38	C
ATOM	4427	CA	PRO	A	565	30.281	8.152	4.256	1.00	62.68	C
ATOM	4428	CB	PRO	A	565	29.970	7.416	2.959	1.00	65.77	C
ATOM	4429	CG	PRO	A	565	28.610	7.980	2.593	1.00	66.19	C
ATOM	4430	C	PRO	A	565	31.771	8.362	4.479	1.00	58.90	C
ATOM	4431	O	PRO	A	565	32.416	9.096	3.725	1.00	56.35	O
ATOM	4432	N	TRP	A	566	32.303	7.735	5.528	1.00	55.77	N
ATOM	4433	CA	TRP	A	566	33.716	7.874	5.874	1.00	47.51	C
ATOM	4434	CB	TRP	A	566	34.080	6.997	7.066	1.00	43.76	C
ATOM	4435	CG	TRP	A	566	33.809	5.534	6.907	1.00	38.32	C
ATOM	4436	CD2	TRP	A	566	34.698	4.556	6.364	1.00	33.14	C
ATOM	4437	CE2	TRP	A	566	34.087	3.308	6.516	1.00	32.56	C
ATOM	4438	CE3	TRP	A	566	35.958	4.618	5.767	1.00	31.48	C
ATOM	4439	CD1	TRP	A	566	32.712	4.850	7.345	1.00	37.64	C
ATOM	4440	NE1	TRP	A	566	32.873	3.510	7.118	1.00	34.21	N
ATOM	4441	CZ2	TRP	A	566	34.690	2.143	6.095	1.00	28.09	C
ATOM	4442	CZ3	TRP	A	566	36.544	3.467	5.352	1.00	23.23	C
ATOM	4443	CH2	TRP	A	566	35.918	2.249	5.516	1.00	25.82	C
ATOM	4444	C	TRP	A	566	34.595	7.529	4.710	1.00	45.07	C
ATOM	4445	O	TRP	A	566	35.671	8.101	4.544	1.00	39.86	O
ATOM	4446	N	THR	A	567	34.120	6.590	3.899	1.00	44.81	N
ATOM	4447	CA	THR	A	567	34.852	6.164	2.717	1.00	45.14	C
ATOM	4448	CB	THR	A	567	34.075	5.048	1.989	1.00	41.05	C
ATOM	4449	OG1	THR	A	567	33.804	5.443	0.644	1.00	44.03	O
ATOM	4450	CG2	THR	A	567	32.787	4.773	2.693	1.00	37.28	C
ATOM	4451	C	THR	A	567	35.092	7.375	1.799	1.00	45.33	C
ATOM	4452	O	THR	A	567	36.201	7.613	1.340	1.00	44.21	O
ATOM	4453	N	LEU	A	568	34.050	8.155	1.549	1.00	49.22	N
ATOM	4454	CA	LEU	A	568	34.193	9.340	0.716	1.00	52.55	C
ATOM	4455	CB	LEU	A	568	32.832	10.010	0.492	1.00	53.15	C
ATOM	4456	CG	LEU	A	568	32.660	11.083	-0.590	1.00	48.21	C
ATOM	4457	CD1	LEU	A	568	31.400	11.848	-0.279	1.00	46.56	C
ATOM	4458	CD2	LEU	A	568	33.826	12.031	-0.629	1.00	44.55	C
ATOM	4459	C	LEU	A	568	35.089	10.293	1.483	1.00	55.12	C
ATOM	4460	O	LEU	A	568	36.138	10.706	0.992	1.00	57.15	O
ATOM	4461	N	ALA	A	569	34.652	10.635	2.694	1.00	55.22	N
ATOM	4462	CA	ALA	A	569	35.383	11.545	3.561	1.00	56.08	C
ATOM	4463	CB	ALA	A	569	34.869	11.430	4.965	1.00	55.88	C
ATOM	4464	C	ALA	A	569	36.866	11.256	3.541	1.00	57.21	C
ATOM	4465	O	ALA	A	569	37.676	12.129	3.251	1.00	57.53	O
ATOM	4466	N	LEU	A	570	37.216	10.018	3.859	1.00	58.29	N
ATOM	4467	CA	LEU	A	570	38.608	9.601	3.882	1.00	58.54	C
ATOM	4468	CB	LEU	A	570	38.678	8.081	4.042	1.00	57.43	C
ATOM	4469	CG	LEU	A	570	39.892	7.432	4.697	1.00	52.56	C
ATOM	4470	CD1	LEU	A	570	39.570	5.994	4.964	1.00	49.23	C
ATOM	4471	CD2	LEU	A	570	41.093	7.552	3.807	1.00	52.68	C
ATOM	4472	C	LEU	A	570	39.228	10.031	2.566	1.00	59.42	C
ATOM	4473	O	LEU	A	570	40.177	10.812	2.543	1.00	59.21	O
ATOM	4474	N	GLU	A	571	38.647	9.535	1.475	1.00	61.82	N
ATOM	4475	CA	GLU	A	571	39.092	9.827	0.112	1.00	63.93	C
ATOM	4476	CB	GLU	A	571	38.040	9.335	-0.883	1.00	63.12	C
ATOM	4477	CG	GLU	A	571	38.607	8.692	-2.138	1.00	66.09	C
ATOM	4478	CD	GLU	A	571	38.146	9.379	-3.407	1.00	68.81	C

370/396

Figure 3B-81

ATOM	4479	OE1	GLU	A	571	38.727	10.430	-3.762	1.00	69.79	O
ATOM	4480	OE2	GLU	A	571	37.195	8.870	-4.042	1.00	68.00	O
ATOM	4481	C	GLU	A	571	39.368	11.313	-0.132	1.00	64.91	C
ATOM	4482	O	GLU	A	571	40.397	11.688	-0.698	1.00	63.36	O
ATOM	4483	N	ASN	A	572	38.441	12.161	0.294	1.00	67.68	N
ATOM	4484	CA	ASN	A	572	38.601	13.598	0.117	1.00	70.76	C
ATOM	4485	CB	ASN	A	572	37.305	14.324	0.472	1.00	70.90	C
ATOM	4486	CG	ASN	A	572	36.418	14.518	-0.718	1.00	71.21	C
ATOM	4487	OD1	ASN	A	572	35.923	13.558	-1.294	1.00	73.70	O
ATOM	4488	ND2	ASN	A	572	36.222	15.769	-1.110	1.00	72.60	N
ATOM	4489	C	ASN	A	572	39.743	14.186	0.940	1.00	72.43	C
ATOM	4490	O	ASN	A	572	40.203	15.302	0.667	1.00	74.92	O
ATOM	4491	N	VAL	A	573	40.200	13.444	1.947	1.00	70.31	N
ATOM	4492	CA	VAL	A	573	41.271	13.931	2.793	1.00	65.94	C
ATOM	4493	CB	VAL	A	573	41.036	13.561	4.253	1.00	62.03	C
ATOM	4494	CG1	VAL	A	573	41.979	14.340	5.130	1.00	62.13	C
ATOM	4495	CG2	VAL	A	573	39.614	13.846	4.634	1.00	63.33	C
ATOM	4496	C	VAL	A	573	42.602	13.359	2.364	1.00	66.59	C
ATOM	4497	O	VAL	A	573	43.513	14.102	1.987	1.00	69.62	O
ATOM	4498	N	VAL	A	574	42.699	12.035	2.408	1.00	65.16	N
ATOM	4499	CA	VAL	A	574	43.927	11.328	2.055	1.00	65.18	C
ATOM	4500	CB	VAL	A	574	44.504	10.565	3.289	1.00	62.86	C
ATOM	4501	CG1	VAL	A	574	44.632	11.504	4.475	1.00	59.47	C
ATOM	4502	CG2	VAL	A	574	43.608	9.403	3.660	1.00	58.91	C
ATOM	4503	C	VAL	A	574	43.669	10.323	0.943	1.00	67.72	C
ATOM	4504	O	VAL	A	574	42.953	9.332	1.145	1.00	70.05	O
ATOM	4505	N	GLY	A	575	44.247	10.580	-0.228	1.00	66.70	N
ATOM	4506	CA	GLY	A	575	44.067	9.688	-1.371	1.00	66.48	C
ATOM	4507	C	GLY	A	575	43.028	8.572	-1.258	1.00	64.75	C
ATOM	4508	O	GLY	A	575	41.865	8.755	-1.607	1.00	63.58	O
ATOM	4509	N	ALA	A	576	43.451	7.412	-0.763	1.00	63.01	N
ATOM	4510	CA	ALA	A	576	42.569	6.257	-0.617	1.00	61.03	C
ATOM	4511	CB	ALA	A	576	43.267	5.174	0.194	1.00	62.87	C
ATOM	4512	C	ALA	A	576	41.206	6.543	-0.006	1.00	59.66	C
ATOM	4513	O	ALA	A	576	41.002	7.570	0.639	1.00	58.05	O
ATOM	4514	N	LYS	A	577	40.286	5.600	-0.218	1.00	58.90	N
ATOM	4515	CA	LYS	A	577	38.919	5.667	0.283	1.00	57.09	C
ATOM	4516	CB	LYS	A	577	37.918	5.688	-0.869	1.00	54.48	C
ATOM	4517	CG	LYS	A	577	37.919	4.407	-1.685	1.00	56.37	C
ATOM	4518	CD	LYS	A	577	36.508	3.862	-1.899	1.00	55.12	C
ATOM	4519	CE	LYS	A	577	35.786	4.544	-3.054	1.00	53.66	C
ATOM	4520	NZ	LYS	A	577	36.332	4.165	-4.386	1.00	41.58	N
ATOM	4521	C	LYS	A	577	38.655	4.434	1.139	1.00	59.15	C
ATOM	4522	O	LYS	A	577	37.527	3.954	1.238	1.00	59.97	O
ATOM	4523	N	ASN	A	578	39.710	3.905	1.743	1.00	61.51	N
ATOM	4524	CA	ASN	A	578	39.575	2.745	2.611	1.00	61.92	C
ATOM	4525	CB	ASN	A	578	39.311	1.481	1.786	1.00	63.85	C
ATOM	4526	CG	ASN	A	578	39.027	0.263	2.653	1.00	66.49	C
ATOM	4527	OD1	ASN	A	578	38.362	0.358	3.689	1.00	67.53	O
ATOM	4528	ND2	ASN	A	578	39.516	-0.894	2.223	1.00	66.70	N
ATOM	4529	C	ASN	A	578	40.828	2.586	3.465	1.00	60.80	C
ATOM	4530	O	ASN	A	578	41.843	3.234	3.222	1.00	60.62	O
ATOM	4531	N	MET	A	579	40.733	1.731	4.473	1.00	58.21	N
ATOM	4532	CA	MET	A	579	41.818	1.472	5.397	1.00	56.83	C
ATOM	4533	CB	MET	A	579	41.314	0.492	6.436	1.00	59.37	C
ATOM	4534	CG	MET	A	579	42.209	0.291	7.615	1.00	63.67	C

371/396

Figure 3B-82

ATOM	4535	SD	MET	A	579	41.371	-0.795	8.761	1.00	67.40	S
ATOM	4536	CE	MET	A	579	40.870	-2.110	7.628	1.00	67.25	C
ATOM	4537	C	MET	A	579	43.092	0.951	4.727	1.00	57.10	C
ATOM	4538	O	MET	A	579	43.092	-0.085	4.067	1.00	53.06	O
ATOM	4539	N	ASN	A	580	44.184	1.685	4.922	1.00	60.93	N
ATOM	4540	CA	ASN	A	580	45.485	1.349	4.339	1.00	63.34	C
ATOM	4541	CB	ASN	A	580	45.956	2.489	3.429	1.00	67.18	C
ATOM	4542	CG	ASN	A	580	47.219	2.144	2.658	1.00	72.93	C
ATOM	4543	OD1	ASN	A	580	47.779	2.989	1.946	1.00	75.04	O
ATOM	4544	ND2	ASN	A	580	47.672	0.895	2.788	1.00	75.29	N
ATOM	4545	C	ASN	A	580	46.556	1.086	5.398	1.00	62.12	C
ATOM	4546	O	ASN	A	580	46.866	1.952	6.220	1.00	61.20	O
ATOM	4547	N	VAL	A	581	47.136	-0.106	5.349	1.00	59.69	N
ATOM	4548	CA	VAL	A	581	48.164	-0.493	6.298	1.00	56.31	C
ATOM	4549	CB	VAL	A	581	48.258	-2.039	6.401	1.00	51.19	C
ATOM	4550	CG1	VAL	A	581	49.572	-2.526	5.854	1.00	51.54	C
ATOM	4551	CG2	VAL	A	581	48.102	-2.473	7.822	1.00	46.62	C
ATOM	4552	C	VAL	A	581	49.540	0.077	5.945	1.00	56.82	C
ATOM	4553	O	VAL	A	581	50.303	0.440	6.831	1.00	57.47	O
ATOM	4554	N	ARG	A	582	49.845	0.184	4.657	1.00	57.10	N
ATOM	4555	CA	ARG	A	582	51.152	0.671	4.227	1.00	61.40	C
ATOM	4556	CB	ARG	A	582	51.226	0.712	2.698	1.00	66.45	C
ATOM	4557	CG	ARG	A	582	51.886	-0.508	2.057	1.00	71.24	C
ATOM	4558	CD	ARG	A	582	50.988	-1.750	2.081	1.00	80.36	C
ATOM	4559	NE	ARG	A	582	49.704	-1.544	1.389	1.00	88.06	N
ATOM	4560	CZ	ARG	A	582	49.023	-2.492	0.737	1.00	88.11	C
ATOM	4561	NH1	ARG	A	582	49.495	-3.733	0.666	1.00	87.68	N
ATOM	4562	NH2	ARG	A	582	47.860	-2.203	0.157	1.00	86.29	N
ATOM	4563	C	ARG	A	582	51.706	1.987	4.782	1.00	62.03	C
ATOM	4564	O	ARG	A	582	52.883	2.062	5.111	1.00	61.15	O
ATOM	4565	N	PRO	A	583	50.893	3.048	4.881	1.00	64.06	N
ATOM	4566	CD	PRO	A	583	49.439	3.252	4.768	1.00	66.39	C
ATOM	4567	CA	PRO	A	583	51.551	4.241	5.426	1.00	64.64	C
ATOM	4568	CB	PRO	A	583	50.443	5.299	5.404	1.00	63.06	C
ATOM	4569	CG	PRO	A	583	49.218	4.490	5.644	1.00	67.02	C
ATOM	4570	C	PRO	A	583	52.103	3.969	6.828	1.00	63.26	C
ATOM	4571	O	PRO	A	583	53.023	4.654	7.286	1.00	63.86	O
ATOM	4572	N	LEU	A	584	51.542	2.969	7.503	1.00	60.57	N
ATOM	4573	CA	LEU	A	584	52.023	2.615	8.831	1.00	60.55	C
ATOM	4574	CB	LEU	A	584	51.004	1.749	9.584	1.00	57.11	C
ATOM	4575	CG	LEU	A	584	51.431	1.304	10.988	1.00	52.51	C
ATOM	4576	CD1	LEU	A	584	50.226	0.969	11.834	1.00	49.66	C
ATOM	4577	CD2	LEU	A	584	52.354	0.109	10.876	1.00	50.52	C
ATOM	4578	C	LEU	A	584	53.339	1.861	8.650	1.00	60.77	C
ATOM	4579	O	LEU	A	584	54.372	2.279	9.172	1.00	64.25	O
ATOM	4580	N	LEU	A	585	53.298	0.760	7.903	1.00	57.82	N
ATOM	4581	CA	LEU	A	585	54.491	-0.035	7.636	1.00	53.71	C
ATOM	4582	CB	LEU	A	585	54.208	-1.058	6.536	1.00	48.54	C
ATOM	4583	CG	LEU	A	585	53.603	-2.389	6.973	1.00	47.29	C
ATOM	4584	CD1	LEU	A	585	52.666	-2.176	8.120	1.00	46.79	C
ATOM	4585	CD2	LEU	A	585	52.894	-3.037	5.796	1.00	50.46	C
ATOM	4586	C	LEU	A	585	55.647	0.861	7.216	1.00	54.82	C
ATOM	4587	O	LEU	A	585	56.808	0.510	7.397	1.00	55.59	O
ATOM	4588	N	ASN	A	586	55.322	2.020	6.654	1.00	57.08	N
ATOM	4589	CA	ASN	A	586	56.330	2.976	6.214	1.00	60.23	C
ATOM	4590	CB	ASN	A	586	55.699	4.016	5.289	1.00	64.88	C

372/396

Figure 3B-83

ATOM	4591	CG	ASN	A	586	55.809	3.640	3.821	1.00	69.74	C
ATOM	4592	OD1	ASN	A	586	55.125	4.215	2.966	1.00	74.48	O
ATOM	4593	ND2	ASN	A	586	56.681	2.684	3.518	1.00	69.60	N
ATOM	4594	C	ASN	A	586	56.931	3.676	7.419	1.00	59.57	C
ATOM	4595	O	ASN	A	586	58.143	3.889	7.499	1.00	56.98	O
ATOM	4596	N	TYR	A	587	56.058	4.041	8.348	1.00	59.52	N
ATOM	4597	CA	TYR	A	587	56.463	4.712	9.574	1.00	60.77	C
ATOM	4598	CB	TYR	A	587	55.257	4.875	10.493	1.00	58.84	C
ATOM	4599	CG	TYR	A	587	55.458	5.806	11.664	1.00	56.90	C
ATOM	4600	CD1	TYR	A	587	55.122	7.134	11.570	1.00	56.79	C
ATOM	4601	CE1	TYR	A	587	55.224	7.963	12.655	1.00	58.05	C
ATOM	4602	CD2	TYR	A	587	55.918	5.337	12.883	1.00	56.51	C
ATOM	4603	CE2	TYR	A	587	56.028	6.161	13.975	1.00	53.41	C
ATOM	4604	CZ	TYR	A	587	55.671	7.475	13.856	1.00	55.26	C
ATOM	4605	OH	TYR	A	587	55.705	8.314	14.942	1.00	56.62	O
ATOM	4606	C	TYR	A	587	57.495	3.840	10.273	1.00	61.58	C
ATOM	4607	O	TYR	A	587	58.564	4.299	10.665	1.00	64.71	O
ATOM	4608	N	PHE	A	588	57.164	2.568	10.409	1.00	59.60	N
ATOM	4609	CA	PHE	A	588	58.029	1.636	11.088	1.00	59.41	C
ATOM	4610	CB	PHE	A	588	57.180	0.645	11.877	1.00	55.57	C
ATOM	4611	CG	PHE	A	588	56.382	1.268	12.974	1.00	49.09	C
ATOM	4612	CD1	PHE	A	588	55.154	0.766	13.313	1.00	46.55	C
ATOM	4613	CD2	PHE	A	588	56.872	2.339	13.680	1.00	52.26	C
ATOM	4614	CE1	PHE	A	588	54.423	1.314	14.330	1.00	47.03	C
ATOM	4615	CE2	PHE	A	588	56.141	2.894	14.706	1.00	52.39	C
ATOM	4616	CZ	PHE	A	588	54.911	2.376	15.028	1.00	49.65	C
ATOM	4617	C	PHE	A	588	58.986	0.860	10.203	1.00	64.09	C
ATOM	4618	O	PHE	A	588	59.498	-0.167	10.638	1.00	68.71	O
ATOM	4619	N	GLU	A	589	59.242	1.301	8.975	1.00	67.04	N
ATOM	4620	CA	GLU	A	589	60.185	0.538	8.150	1.00	69.27	C
ATOM	4621	CB	GLU	A	589	60.214	1.026	6.699	1.00	71.79	C
ATOM	4622	CG	GLU	A	589	59.315	0.219	5.749	1.00	75.41	C
ATOM	4623	CD	GLU	A	589	59.374	-1.295	5.983	1.00	77.44	C
ATOM	4624	OE1	GLU	A	589	58.467	-1.818	6.676	1.00	75.92	O
ATOM	4625	OE2	GLU	A	589	60.320	-1.955	5.481	1.00	75.42	O
ATOM	4626	C	GLU	A	589	61.598	0.574	8.725	1.00	68.63	C
ATOM	4627	O	GLU	A	589	62.302	-0.437	8.703	1.00	69.32	O
ATOM	4628	N	PRO	A	590	62.036	1.740	9.244	1.00	66.74	N
ATOM	4629	CD	PRO	A	590	61.384	3.060	9.174	1.00	64.45	C
ATOM	4630	CA	PRO	A	590	63.380	1.860	9.826	1.00	64.47	C
ATOM	4631	CB	PRO	A	590	63.437	3.322	10.264	1.00	64.17	C
ATOM	4632	CG	PRO	A	590	62.561	3.998	9.276	1.00	64.56	C
ATOM	4633	C	PRO	A	590	63.560	0.896	11.000	1.00	61.91	C
ATOM	4634	O	PRO	A	590	64.508	0.122	11.045	1.00	61.60	O
ATOM	4635	N	LEU	A	591	62.631	0.961	11.944	1.00	61.55	N
ATOM	4636	CA	LEU	A	591	62.635	0.106	13.118	1.00	62.11	C
ATOM	4637	CB	LEU	A	591	61.466	0.464	14.030	1.00	64.32	C
ATOM	4638	CG	LEU	A	591	61.096	-0.573	15.090	1.00	65.16	C
ATOM	4639	CD1	LEU	A	591	62.231	-0.736	16.087	1.00	68.06	C
ATOM	4640	CD2	LEU	A	591	59.850	-0.117	15.797	1.00	66.71	C
ATOM	4641	C	LEU	A	591	62.516	-1.361	12.750	1.00	61.53	C
ATOM	4642	O	LEU	A	591	63.107	-2.214	13.397	1.00	65.14	O
ATOM	4643	N	PHE	A	592	61.735	-1.654	11.722	1.00	57.90	N
ATOM	4644	CA	PHE	A	592	61.540	-3.027	11.295	1.00	56.25	C
ATOM	4645	CB	PHE	A	592	60.509	-3.062	10.180	1.00	49.57	C
ATOM	4646	CG	PHE	A	592	60.132	-4.443	9.737	1.00	44.76	C

373/396

Figure 3B-84

ATOM	4647	CD1	PHE	A	592	59.539	-5.328	10.614	1.00	46.72	C
ATOM	4648	CD2	PHE	A	592	60.313	-4.833	8.424	1.00	41.67	C
ATOM	4649	CE1	PHE	A	592	59.129	-6.575	10.188	1.00	43.18	C
ATOM	4650	CE2	PHE	A	592	59.909	-6.065	7.999	1.00	39.29	C
ATOM	4651	CZ	PHE	A	592	59.314	-6.937	8.881	1.00	42.50	C
ATOM	4652	C	PHE	A	592	62.840	-3.670	10.817	1.00	60.91	C
ATOM	4653	O	PHE	A	592	63.247	-4.712	11.322	1.00	61.94	O
ATOM	4654	N	THR	A	593	63.496	-3.044	9.846	1.00	65.01	N
ATOM	4655	CA	THR	A	593	64.737	-3.582	9.300	1.00	68.16	C
ATOM	4656	CB	THR	A	593	65.262	-2.694	8.123	1.00	65.93	C
ATOM	4657	OG1	THR	A	593	65.231	-1.311	8.490	1.00	63.19	O
ATOM	4658	CG2	THR	A	593	64.397	-2.886	6.890	1.00	65.51	C
ATOM	4659	C	THR	A	593	65.833	-3.786	10.355	1.00	72.36	C
ATOM	4660	O	THR	A	593	66.624	-4.729	10.249	1.00	73.31	O
ATOM	4661	N	TRP	A	594	65.869	-2.909	11.363	1.00	74.42	N
ATOM	4662	CA	TRP	A	594	66.841	-2.974	12.465	1.00	76.14	C
ATOM	4663	CB	TRP	A	594	66.845	-1.645	13.230	1.00	77.58	C
ATOM	4664	CG	TRP	A	594	67.663	-1.572	14.522	1.00	78.77	C
ATOM	4665	CD2	TRP	A	594	67.254	-1.996	15.834	1.00	78.85	C
ATOM	4666	CE2	TRP	A	594	68.263	-1.600	16.737	1.00	78.86	C
ATOM	4667	CE3	TRP	A	594	66.134	-2.667	16.330	1.00	78.69	C
ATOM	4668	CD1	TRP	A	594	68.877	-0.962	14.688	1.00	80.24	C
ATOM	4669	NE1	TRP	A	594	69.240	-0.969	16.016	1.00	79.43	N
ATOM	4670	CZ2	TRP	A	594	68.179	-1.848	18.104	1.00	78.12	C
ATOM	4671	CZ3	TRP	A	594	66.055	-2.912	17.688	1.00	78.96	C
ATOM	4672	CH2	TRP	A	594	67.072	-2.504	18.559	1.00	77.85	C
ATOM	4673	C	TRP	A	594	66.389	-4.096	13.389	1.00	77.54	C
ATOM	4674	O	TRP	A	594	67.204	-4.833	13.939	1.00	79.28	O
ATOM	4675	N	LEU	A	595	65.073	-4.200	13.558	1.00	77.16	N
ATOM	4676	CA	LEU	A	595	64.467	-5.230	14.389	1.00	76.42	C
ATOM	4677	CB	LEU	A	595	62.948	-5.094	14.369	1.00	74.45	C
ATOM	4678	CG	LEU	A	595	62.215	-5.206	15.696	1.00	72.81	C
ATOM	4679	CD1	LEU	A	595	62.595	-4.027	16.558	1.00	72.97	C
ATOM	4680	CD2	LEU	A	595	60.724	-5.219	15.462	1.00	73.46	C
ATOM	4681	C	LEU	A	595	64.855	-6.538	13.732	1.00	78.79	C
ATOM	4682	O	LEU	A	595	64.953	-7.574	14.380	1.00	79.74	O
ATOM	4683	N	LYS	A	596	65.053	-6.478	12.420	1.00	81.24	N
ATOM	4684	CA	LYS	A	596	65.447	-7.649	11.658	1.00	82.87	C
ATOM	4685	CB	LYS	A	596	65.515	-7.306	10.167	1.00	81.64	C
ATOM	4686	CG	LYS	A	596	64.186	-6.832	9.564	1.00	81.13	C
ATOM	4687	CD	LYS	A	596	63.215	-7.980	9.256	1.00	77.11	C
ATOM	4688	CE	LYS	A	596	63.224	-8.362	7.770	1.00	74.52	C
ATOM	4689	NZ	LYS	A	596	62.872	-7.222	6.870	1.00	68.76	N
ATOM	4690	C	LYS	A	596	66.822	-8.044	12.181	1.00	85.21	C
ATOM	4691	O	LYS	A	596	66.999	-9.141	12.712	1.00	84.55	O
ATOM	4692	N	ASP	A	597	67.785	-7.133	12.047	1.00	87.83	N
ATOM	4693	CA	ASP	A	597	69.142	-7.378	12.523	1.00	89.83	C
ATOM	4694	CB	ASP	A	597	69.990	-6.102	12.444	1.00	94.14	C
ATOM	4695	CG	ASP	A	597	70.623	-5.903	11.065	1.00	101.54	C
ATOM	4696	OD1	ASP	A	597	71.441	-6.762	10.664	1.00	104.43	O
ATOM	4697	OD2	ASP	A	597	70.307	-4.899	10.377	1.00	104.00	O
ATOM	4698	C	ASP	A	597	69.095	-7.887	13.951	1.00	89.53	C
ATOM	4699	O	ASP	A	597	69.182	-9.084	14.179	1.00	91.24	O
ATOM	4700	N	GLN	A	598	68.938	-6.984	14.911	1.00	87.21	N
ATOM	4701	CA	GLN	A	598	68.882	-7.372	16.315	1.00	84.30	C
ATOM	4702	CB	GLN	A	598	68.034	-6.380	17.094	1.00	85.23	C

374/396

Figure 3B-85

ATOM	4703	CG	GLN	A	598	68.578	-4.973	17.067	1.00	86.82	C
ATOM	4704	CD	GLN	A	598	69.915	-4.859	17.755	1.00	87.89	C
ATOM	4705	OE1	GLN	A	598	70.058	-5.227	18.922	1.00	87.64	O
ATOM	4706	NE2	GLN	A	598	70.907	-4.344	17.037	1.00	87.80	N
ATOM	4707	C	GLN	A	598	68.343	-8.780	16.540	1.00	83.38	C
ATOM	4708	O	GLN	A	598	68.912	-9.546	17.308	1.00	86.37	O
ATOM	4709	N	ASN	A	599	67.255	-9.130	15.869	1.00	80.82	N
ATOM	4710	CA	ASN	A	599	66.666	-10.454	16.034	1.00	79.55	C
ATOM	4711	CB	ASN	A	599	65.210	-10.447	15.556	1.00	80.80	C
ATOM	4712	CG	ASN	A	599	64.240	-10.014	16.632	1.00	80.80	C
ATOM	4713	OD1	ASN	A	599	63.640	-10.842	17.315	1.00	82.15	O
ATOM	4714	ND2	ASN	A	599	64.083	-8.711	16.792	1.00	82.04	N
ATOM	4715	C	ASN	A	599	67.407	-11.579	15.321	1.00	79.34	C
ATOM	4716	O	ASN	A	599	67.169	-12.742	15.623	1.00	78.54	O
ATOM	4717	N	LYS	A	600	68.289	-11.237	14.380	1.00	80.09	N
ATOM	4718	CA	LYS	A	600	69.054	-12.225	13.599	1.00	81.14	C
ATOM	4719	CB	LYS	A	600	70.354	-11.608	13.062	1.00	79.05	C
ATOM	4720	CG	LYS	A	600	71.247	-11.003	14.126	1.00	79.54	C
ATOM	4721	CD	LYS	A	600	72.229	-10.011	13.524	1.00	77.99	C
ATOM	4722	CE	LYS	A	600	72.903	-9.197	14.614	1.00	77.08	C
ATOM	4723	NZ	LYS	A	600	73.853	-8.215	14.035	1.00	78.54	N
ATOM	4724	C	LYS	A	600	69.382	-13.496	14.358	1.00	82.86	C
ATOM	4725	O	LYS	A	600	69.293	-14.594	13.806	1.00	84.12	O
ATOM	4726	N	ASN	A	601	69.759	-13.335	15.625	1.00	84.52	N
ATOM	4727	CA	ASN	A	601	70.095	-14.456	16.501	1.00	83.61	C
ATOM	4728	CB	ASN	A	601	71.185	-14.030	17.496	1.00	87.74	C
ATOM	4729	CG	ASN	A	601	70.875	-12.699	18.180	1.00	92.86	C
ATOM	4730	OD1	ASN	A	601	69.910	-12.584	18.941	1.00	93.22	O
ATOM	4731	ND2	ASN	A	601	71.698	-11.684	17.904	1.00	95.06	N
ATOM	4732	C	ASN	A	601	68.864	-14.982	17.252	1.00	80.75	C
ATOM	4733	O	ASN	A	601	68.629	-16.190	17.301	1.00	80.47	O
ATOM	4734	N	SER	A	602	68.073	-14.068	17.814	1.00	77.24	N
ATOM	4735	CA	SER	A	602	66.867	-14.422	18.565	1.00	73.43	C
ATOM	4736	CB	SER	A	602	66.332	-13.165	19.261	1.00	72.33	C
ATOM	4737	OG	SER	A	602	65.421	-13.481	20.294	1.00	73.96	O
ATOM	4738	C	SER	A	602	65.784	-15.060	17.667	1.00	71.50	C
ATOM	4739	O	SER	A	602	65.795	-14.887	16.450	1.00	72.00	O
ATOM	4740	N	PHE	A	603	64.855	-15.799	18.270	1.00	68.37	N
ATOM	4741	CA	PHE	A	603	63.785	-16.477	17.530	1.00	67.69	C
ATOM	4742	CB	PHE	A	603	63.338	-17.716	18.280	1.00	63.01	C
ATOM	4743	CG	PHE	A	603	62.145	-18.397	17.674	1.00	58.29	C
ATOM	4744	CD1	PHE	A	603	61.060	-18.754	18.463	1.00	57.24	C
ATOM	4745	CD2	PHE	A	603	62.157	-18.791	16.351	1.00	56.65	C
ATOM	4746	CE1	PHE	A	603	60.015	-19.503	17.946	1.00	54.25	C
ATOM	4747	CE2	PHE	A	603	61.113	-19.543	15.832	1.00	57.00	C
ATOM	4748	CZ	PHE	A	603	60.043	-19.900	16.636	1.00	54.16	C
ATOM	4749	C	PHE	A	603	62.539	-15.645	17.281	1.00	71.17	C
ATOM	4750	O	PHE	A	603	61.939	-15.119	18.225	1.00	73.90	O
ATOM	4751	N	VAL	A	604	62.129	-15.559	16.017	1.00	71.97	N
ATOM	4752	CA	VAL	A	604	60.933	-14.805	15.655	1.00	69.47	C
ATOM	4753	CB	VAL	A	604	61.123	-14.046	14.344	1.00	66.76	C
ATOM	4754	CG1	VAL	A	604	59.796	-13.468	13.904	1.00	68.28	C
ATOM	4755	CG2	VAL	A	604	62.150	-12.935	14.531	1.00	65.74	C
ATOM	4756	C	VAL	A	604	59.727	-15.734	15.531	1.00	70.39	C
ATOM	4757	O	VAL	A	604	59.608	-16.515	14.580	1.00	69.44	O
ATOM	4758	N	GLY	A	605	58.835	-15.631	16.512	1.00	70.32	N

375/396

Figure 3B-86

ATOM	4759	CA	GLY	A	605	57.651	-16.461	16.557	1.00	70.25	C
ATOM	4760	C	GLY	A	605	57.475	-16.912	17.990	1.00	71.49	C
ATOM	4761	O	GLY	A	605	58.296	-16.582	18.845	1.00	72.50	O
ATOM	4762	N	TRP	A	606	56.422	-17.673	18.262	1.00	72.49	N
ATOM	4763	CA	TRP	A	606	56.165	-18.136	19.618	1.00	74.74	C
ATOM	4764	CB	TRP	A	606	55.384	-17.061	20.381	1.00	72.67	C
ATOM	4765	CG	TRP	A	606	54.059	-16.670	19.729	1.00	70.69	C
ATOM	4766	CD2	TRP	A	606	53.769	-15.445	19.049	1.00	65.18	C
ATOM	4767	CE2	TRP	A	606	52.432	-15.513	18.606	1.00	62.78	C
ATOM	4768	CE3	TRP	A	606	54.512	-14.296	18.772	1.00	61.66	C
ATOM	4769	CD1	TRP	A	606	52.905	-17.418	19.668	1.00	69.47	C
ATOM	4770	NE1	TRP	A	606	51.926	-16.726	18.994	1.00	63.42	N
ATOM	4771	CZ2	TRP	A	606	51.829	-14.481	17.906	1.00	62.11	C
ATOM	4772	CZ3	TRP	A	606	53.911	-13.274	18.078	1.00	62.81	C
ATOM	4773	CH2	TRP	A	606	52.582	-13.370	17.651	1.00	62.25	C
ATOM	4774	C	TRP	A	606	55.391	-19.449	19.634	1.00	78.50	C
ATOM	4775	O	TRP	A	606	54.784	-19.834	18.631	1.00	77.05	O
ATOM	4776	N	SER	A	607	55.413	-20.123	20.785	1.00	83.35	N
ATOM	4777	CA	SER	A	607	54.718	-21.399	20.966	1.00	88.13	C
ATOM	4778	CB	SER	A	607	55.557	-22.350	21.820	1.00	90.00	C
ATOM	4779	OG	SER	A	607	54.789	-23.481	22.213	1.00	92.95	O
ATOM	4780	C	SER	A	607	53.342	-21.264	21.612	1.00	89.56	C
ATOM	4781	O	SER	A	607	53.183	-20.602	22.636	1.00	90.10	O
ATOM	4782	N	THR	A	608	52.358	-21.924	21.014	1.00	90.92	N
ATOM	4783	CA	THR	A	608	50.993	-21.900	21.510	1.00	93.68	C
ATOM	4784	CB	THR	A	608	49.993	-21.969	20.337	1.00	93.23	C
ATOM	4785	OG1	THR	A	608	48.657	-22.050	20.844	1.00	93.77	O
ATOM	4786	CG2	THR	A	608	50.279	-23.185	19.466	1.00	92.69	C
ATOM	4787	C	THR	A	608	50.745	-23.078	22.456	1.00	96.58	C
ATOM	4788	O	THR	A	608	49.597	-23.440	22.725	1.00	96.87	O
ATOM	4789	N	ASP	A	609	51.825	-23.672	22.959	1.00	99.24	N
ATOM	4790	CA	ASP	A	609	51.719	-24.811	23.869	1.00	102.31	C
ATOM	4791	CB	ASP	A	609	52.190	-26.103	23.182	1.00	105.10	C
ATOM	4792	CG	ASP	A	609	51.108	-26.749	22.319	1.00	108.02	C
ATOM	4793	OD1	ASP	A	609	50.769	-26.190	21.251	1.00	109.83	O
ATOM	4794	OD2	ASP	A	609	50.596	-27.823	22.713	1.00	107.36	O
ATOM	4795	C	ASP	A	609	52.520	-24.613	25.149	1.00	102.52	C
ATOM	4796	O	ASP	A	609	52.366	-25.374	26.105	1.00	102.10	O
ATOM	4797	N	TRP	A	610	53.372	-23.592	25.160	1.00	103.47	N
ATOM	4798	CA	TRP	A	610	54.215	-23.286	26.314	1.00	105.10	C
ATOM	4799	CB	TRP	A	610	54.971	-21.964	26.082	1.00	106.08	C
ATOM	4800	CG	TRP	A	610	56.093	-21.710	27.064	1.00	105.47	C
ATOM	4801	CD2	TRP	A	610	56.156	-20.677	28.057	1.00	105.55	C
ATOM	4802	CE2	TRP	A	610	57.357	-20.855	28.768	1.00	106.07	C
ATOM	4803	CE3	TRP	A	610	55.314	-19.622	28.415	1.00	106.04	C
ATOM	4804	CD1	TRP	A	610	57.229	-22.445	27.209	1.00	105.93	C
ATOM	4805	NE1	TRP	A	610	57.994	-21.941	28.230	1.00	105.97	N
ATOM	4806	CZ2	TRP	A	610	57.740	-20.017	29.816	1.00	105.88	C
ATOM	4807	CZ3	TRP	A	610	55.696	-18.791	29.458	1.00	107.68	C
ATOM	4808	CH2	TRP	A	610	56.900	-18.996	30.145	1.00	105.72	C
ATOM	4809	C	TRP	A	610	53.423	-23.191	27.619	1.00	106.18	C
ATOM	4810	O	TRP	A	610	52.376	-23.819	27.777	1.00	105.92	O
ATOM	4811	N	SER	A	611	53.951	-22.392	28.544	1.00	107.88	N
ATOM	4812	CA	SER	A	611	53.359	-22.158	29.858	1.00	108.88	C
ATOM	4813	CB	SER	A	611	52.706	-23.439	30.390	1.00	108.56	C
ATOM	4814	OG	SER	A	611	52.113	-23.224	31.655	1.00	109.20	O

376/396

Figure 3B-87

ATOM	4815	C	SER	A	611	54.448	-21.691	30.831	1.00	108.90	C
ATOM	4816	O	SER	A	611	55.564	-22.217	30.830	1.00	108.21	O
ATOM	4817	N	PRO	A	612	54.144	-20.668	31.646	1.00	109.32	N
ATOM	4818	CD	PRO	A	612	53.016	-19.743	31.429	1.00	109.45	C
ATOM	4819	CA	PRO	A	612	55.080	-20.119	32.632	1.00	110.10	C
ATOM	4820	CB	PRO	A	612	54.689	-18.650	32.681	1.00	110.25	C
ATOM	4821	CG	PRO	A	612	53.204	-18.720	32.538	1.00	110.16	C
ATOM	4822	C	PRO	A	612	54.926	-20.803	33.995	1.00	110.88	C
ATOM	4823	O	PRO	A	612	55.903	-21.010	34.721	1.00	109.90	O
ATOM	4824	N	TYR	A	613	53.690	-21.152	34.335	1.00	111.78	N
ATOM	4825	CA	TYR	A	613	53.417	-21.808	35.604	1.00	112.51	C
ATOM	4826	CB	TYR	A	613	51.953	-21.590	36.019	1.00	110.29	C
ATOM	4827	CG	TYR	A	613	50.900	-21.893	34.969	1.00	107.21	C
ATOM	4828	CD1	TYR	A	613	50.377	-23.172	34.818	1.00	106.87	C
ATOM	4829	CE1	TYR	A	613	49.365	-23.431	33.908	1.00	106.05	C
ATOM	4830	CD2	TYR	A	613	50.384	-20.885	34.172	1.00	107.28	C
ATOM	4831	CE2	TYR	A	613	49.375	-21.135	33.260	1.00	107.04	C
ATOM	4832	CZ	TYR	A	613	48.867	-22.404	33.132	1.00	106.65	C
ATOM	4833	OH	TYR	A	613	47.847	-22.634	32.234	1.00	105.69	O
ATOM	4834	C	TYR	A	613	53.759	-23.290	35.551	1.00	113.99	C
ATOM	4835	O	TYR	A	613	52.849	-24.134	35.697	1.00	114.94	O
ATOM	4836	OXT	TYR	A	613	54.958	-23.582	35.361	1.00	114.71	O
TER	4837		TYR	A	613					A	
ATOM	4838	CB	ALA	A	614	51.550	-27.785	33.567	1.00	131.92	C
ATOM	4839	C	ALA	A	614	53.907	-27.072	34.012	1.00	132.24	C
ATOM	4840	O	ALA	A	614	54.209	-28.256	33.847	1.00	132.12	O
ATOM	4841	N	ALA	A	614	52.351	-25.626	32.709	1.00	130.34	N
ATOM	4842	CA	ALA	A	614	52.462	-26.599	33.830	1.00	131.49	C
ATOM	4843	N	ASP	A	615	54.791	-26.137	34.353	1.00	132.65	N
ATOM	4844	CA	ASP	A	615	56.209	-26.432	34.564	1.00	132.29	C
ATOM	4845	CB	ASP	A	615	57.033	-25.141	34.462	1.00	133.11	C
ATOM	4846	CG	ASP	A	615	58.503	-25.353	34.777	1.00	133.01	C
ATOM	4847	OD1	ASP	A	615	59.154	-26.159	34.080	1.00	133.23	O
ATOM	4848	OD2	ASP	A	615	59.005	-24.709	35.723	1.00	132.23	O
ATOM	4849	C	ASP	A	615	56.439	-27.082	35.923	1.00	131.98	C
ATOM	4850	O	ASP	A	615	57.575	-27.194	36.385	1.00	130.94	O
ATOM	4851	N	GLN	A	616	55.352	-27.506	36.561	1.00	132.00	N
ATOM	4852	CA	GLN	A	616	55.424	-28.154	37.866	1.00	131.48	C
ATOM	4853	CB	GLN	A	616	55.605	-27.117	38.974	1.00	131.60	C
ATOM	4854	CG	GLN	A	616	57.036	-26.652	39.161	1.00	132.55	C
ATOM	4855	CD	GLN	A	616	57.170	-25.635	40.271	1.00	133.52	C
ATOM	4856	OE1	GLN	A	616	56.764	-25.882	41.409	1.00	132.89	O
ATOM	4857	NE2	GLN	A	616	57.743	-24.480	39.947	1.00	134.67	N
ATOM	4858	C	GLN	A	616	54.190	-28.991	38.157	1.00	130.86	C
ATOM	4859	O	GLN	A	616	54.219	-29.869	39.021	1.00	131.87	O
ATOM	4860	N	SER	A	617	53.107	-28.720	37.436	1.00	130.09	N
ATOM	4861	CA	SER	A	617	51.863	-29.458	37.625	1.00	129.92	C
ATOM	4862	CB	SER	A	617	50.829	-29.026	36.580	1.00	129.58	C
ATOM	4863	OG	SER	A	617	50.740	-27.616	36.491	1.00	127.66	O
ATOM	4864	C	SER	A	617	52.117	-30.960	37.490	1.00	129.75	C
ATOM	4865	O	SER	A	617	53.245	-31.394	37.249	1.00	129.87	O
ATOM	4866	N	ILE	A	618	51.065	-31.752	37.659	1.00	128.80	N
ATOM	4867	CA	ILE	A	618	51.174	-33.198	37.533	1.00	127.55	C
ATOM	4868	CB	ILE	A	618	51.218	-33.885	38.906	1.00	126.77	C
ATOM	4869	CG2	ILE	A	618	50.863	-35.351	38.753	1.00	127.65	C
ATOM	4870	CG1	ILE	A	618	52.610	-33.735	39.527	1.00	125.91	C

377/396

Figure 3B-88

ATOM	4871	CD1	ILE	A	618	52.925	-32.355	40.053	1.00	123.90	C
ATOM	4872	C	ILE	A	618	49.989	-33.739	36.740	1.00	127.53	C
ATOM	4873	O	ILE	A	618	48.880	-33.868	37.262	1.00	127.25	O
ATOM	4874	N	LYS	A	619	50.245	-34.053	35.473	1.00	127.07	N
ATOM	4875	CA	LYS	A	619	49.228	-34.558	34.558	1.00	126.67	C
ATOM	4876	CB	LYS	A	619	49.889	-35.100	33.285	1.00	124.62	C
ATOM	4877	CG	LYS	A	619	50.345	-34.008	32.328	1.00	123.16	C
ATOM	4878	CD	LYS	A	619	50.929	-34.559	31.033	1.00	120.51	C
ATOM	4879	CE	LYS	A	619	52.297	-35.177	31.254	1.00	118.02	C
ATOM	4880	NZ	LYS	A	619	52.910	-35.589	29.968	1.00	114.88	N
ATOM	4881	C	LYS	A	619	48.285	-35.608	35.121	1.00	128.07	C
ATOM	4882	O	LYS	A	619	48.554	-36.224	36.153	1.00	126.88	O
ATOM	4883	N	VAL	A	620	47.166	-35.783	34.420	1.00	130.70	N
ATOM	4884	CA	VAL	A	620	46.117	-36.745	34.761	1.00	133.30	C
ATOM	4885	CB	VAL	A	620	45.556	-36.506	36.184	1.00	133.57	C
ATOM	4886	CG1	VAL	A	620	46.328	-37.334	37.191	1.00	133.41	C
ATOM	4887	CG2	VAL	A	620	45.655	-35.038	36.546	1.00	134.82	C
ATOM	4888	C	VAL	A	620	44.973	-36.646	33.738	1.00	134.24	C
ATOM	4889	O	VAL	A	620	44.822	-35.626	33.060	1.00	133.84	O
ATOM	4890	N	ALA	A	621	44.170	-37.702	33.629	1.00	134.70	N
ATOM	4891	CA	ALA	A	621	43.074	-37.712	32.664	1.00	134.14	C
ATOM	4892	CB	ALA	A	621	43.357	-38.755	31.578	1.00	134.37	C
ATOM	4893	C	ALA	A	621	41.675	-37.932	33.244	1.00	133.47	C
ATOM	4894	O	ALA	A	621	41.168	-37.098	33.994	1.00	132.12	O
ATOM	4895	N	ALA	A	622	41.063	-39.060	32.877	1.00	132.99	N
ATOM	4896	CA	ALA	A	622	39.706	-39.422	33.295	1.00	131.72	C
ATOM	4897	CB	ALA	A	622	39.487	-39.101	34.770	1.00	131.16	C
ATOM	4898	C	ALA	A	622	38.759	-38.606	32.424	1.00	131.09	C
ATOM	4899	O	ALA	A	622	37.683	-39.064	32.040	1.00	131.47	O
ATOM	4900	N	ALA	A	623	39.205	-37.394	32.111	1.00	130.48	N
ATOM	4901	CA	ALA	A	623	38.493	-36.428	31.279	1.00	129.25	C
ATOM	4902	CB	ALA	A	623	37.203	-35.983	31.959	1.00	129.24	C
ATOM	4903	C	ALA	A	623	39.454	-35.248	31.133	1.00	128.36	C
ATOM	4904	O	ALA	A	623	39.136	-34.241	30.497	1.00	128.06	O
ATOM	4905	N	ALA	A	624	40.628	-35.416	31.750	1.00	127.34	N
ATOM	4906	CA	ALA	A	624	41.734	-34.450	31.772	1.00	125.13	C
ATOM	4907	CB	ALA	A	624	41.563	-33.393	30.666	1.00	125.18	C
ATOM	4908	C	ALA	A	624	41.886	-33.767	33.136	1.00	122.44	C
ATOM	4909	O	ALA	A	624	40.902	-33.558	33.846	1.00	122.57	O
ATOM	4910	N	ALA	A	625	43.124	-33.430	33.495	1.00	118.80	N
ATOM	4911	CA	ALA	A	625	43.420	-32.752	34.759	1.00	114.24	C
ATOM	4912	CB	ALA	A	625	42.946	-33.597	35.936	1.00	113.10	C
ATOM	4913	C	ALA	A	625	44.914	-32.453	34.891	1.00	111.81	C
ATOM	4914	O	ALA	A	625	45.715	-32.849	34.043	1.00	110.99	O
ATOM	4915	N	ALA	A	626	45.286	-31.744	35.951	1.00	109.26	N
ATOM	4916	CA	ALA	A	626	46.686	-31.406	36.176	1.00	107.32	C
ATOM	4917	CB	ALA	A	626	47.172	-30.441	35.096	1.00	107.03	C
ATOM	4918	C	ALA	A	626	46.895	-30.799	37.556	1.00	105.77	C
ATOM	4919	O	ALA	A	626	45.893	-30.585	38.265	1.00	104.03	O
ATOM	4920	OXT	ALA	A	626	48.062	-30.546	37.912	1.00	105.40	O
TER	4921		ALA	A	626					A	
ATOM	4922	CB	ALA	A	661	30.936	-29.517	38.492	1.00	108.02	C
ATOM	4923	C	ALA	A	661	31.957	-30.775	40.399	1.00	109.81	C
ATOM	4924	O	ALA	A	661	33.108	-30.543	40.775	1.00	110.96	O
ATOM	4925	N	ALA	A	661	30.744	-31.973	38.585	1.00	108.68	N
ATOM	4926	CA	ALA	A	661	31.619	-30.814	38.908	1.00	109.23	C

378/396

Figure 3B-89

ATOM	4927	N	ALA	A	662	30.954	-31.003	41.244	1.00	109.19	N
ATOM	4928	CA	ALA	A	662	31.144	-30.992	42.694	1.00	108.24	C
ATOM	4929	CB	ALA	A	662	29.824	-31.308	43.399	1.00	107.62	C
ATOM	4930	C	ALA	A	662	32.219	-31.983	43.133	1.00	107.89	C
ATOM	4931	O	ALA	A	662	32.938	-31.746	44.101	1.00	107.19	O
ATOM	4932	N	ALA	A	663	32.327	-33.097	42.417	1.00	108.60	N
ATOM	4933	CA	ALA	A	663	33.322	-34.110	42.743	1.00	108.47	C
ATOM	4934	CB	ALA	A	663	33.244	-35.263	41.744	1.00	107.87	C
ATOM	4935	C	ALA	A	663	34.718	-33.498	42.732	1.00	108.24	C
ATOM	4936	O	ALA	A	663	35.625	-33.992	43.399	1.00	107.60	O
ATOM	4937	N	ALA	A	664	34.880	-32.415	41.975	1.00	108.49	N
ATOM	4938	CA	ALA	A	664	36.164	-31.729	41.868	1.00	108.55	C
ATOM	4939	CB	ALA	A	664	36.207	-30.913	40.582	1.00	108.85	C
ATOM	4940	C	ALA	A	664	36.451	-30.833	43.082	1.00	109.05	C
ATOM	4941	O	ALA	A	664	37.608	-30.641	43.458	1.00	107.66	O
ATOM	4942	N	ALA	A	665	35.405	-30.280	43.691	1.00	109.10	N
ATOM	4943	CA	ALA	A	665	35.588	-29.439	44.871	1.00	109.53	C
ATOM	4944	CB	ALA	A	665	34.280	-28.768	45.261	1.00	109.91	C
ATOM	4945	C	ALA	A	665	36.054	-30.354	45.991	1.00	110.27	C
ATOM	4946	O	ALA	A	665	36.714	-29.920	46.938	1.00	111.47	O
ATOM	4947	N	ALA	A	666	35.690	-31.629	45.865	1.00	109.72	N
ATOM	4948	CA	ALA	A	666	36.054	-32.656	46.833	1.00	107.85	C
ATOM	4949	CB	ALA	A	666	35.103	-33.846	46.707	1.00	106.43	C
ATOM	4950	C	ALA	A	666	37.498	-33.098	46.590	1.00	106.80	C
ATOM	4951	O	ALA	A	666	38.283	-33.234	47.529	1.00	106.37	O
ATOM	4952	N	ALA	A	667	37.840	-33.321	45.325	1.00	105.51	N
ATOM	4953	CA	ALA	A	667	39.190	-33.729	44.963	1.00	105.10	C
ATOM	4954	CB	ALA	A	667	39.276	-33.997	43.466	1.00	101.51	C
ATOM	4955	C	ALA	A	667	40.112	-32.585	45.347	1.00	106.14	C
ATOM	4956	O	ALA	A	667	41.326	-32.750	45.486	1.00	105.38	O
ATOM	4957	N	ALA	A	668	39.509	-31.416	45.523	1.00	107.76	N
ATOM	4958	CA	ALA	A	668	40.249	-30.221	45.887	1.00	110.06	C
ATOM	4959	CB	ALA	A	668	39.326	-29.015	45.859	1.00	111.48	C
ATOM	4960	C	ALA	A	668	40.843	-30.388	47.272	1.00	111.08	C
ATOM	4961	O	ALA	A	668	42.047	-30.607	47.421	1.00	110.87	O
ATOM	4962	N	ALA	A	669	39.975	-30.286	48.277	1.00	111.82	N
ATOM	4963	CA	ALA	A	669	40.356	-30.410	49.681	1.00	111.24	C
ATOM	4964	CB	ALA	A	669	39.104	-30.482	50.549	1.00	112.24	C
ATOM	4965	C	ALA	A	669	41.239	-31.626	49.939	1.00	110.17	C
ATOM	4966	O	ALA	A	669	42.251	-31.528	50.636	1.00	109.37	O
ATOM	4967	N	ALA	A	670	40.843	-32.769	49.385	1.00	108.79	N
ATOM	4968	CA	ALA	A	670	41.607	-34.000	49.544	1.00	106.97	C
ATOM	4969	CB	ALA	A	670	41.014	-35.095	48.673	1.00	106.83	C
ATOM	4970	C	ALA	A	670	43.057	-33.739	49.152	1.00	106.16	C
ATOM	4971	O	ALA	A	670	43.981	-34.241	49.791	1.00	104.78	O
ATOM	4972	N	ALA	A	671	43.241	-32.940	48.101	1.00	105.70	N
ATOM	4973	CA	ALA	A	671	44.569	-32.582	47.605	1.00	105.63	C
ATOM	4974	CB	ALA	A	671	44.452	-31.984	46.213	1.00	103.21	C
ATOM	4975	C	ALA	A	671	45.229	-31.580	48.549	1.00	106.64	C
ATOM	4976	O	ALA	A	671	46.454	-31.534	48.684	1.00	105.07	O
ATOM	4977	N	ALA	A	672	44.396	-30.776	49.200	1.00	108.72	N
ATOM	4978	CA	ALA	A	672	44.860	-29.766	50.139	1.00	110.19	C
ATOM	4979	CB	ALA	A	672	43.710	-28.837	50.498	1.00	110.44	C
ATOM	4980	C	ALA	A	672	45.420	-30.418	51.399	1.00	111.48	C
ATOM	4981	O	ALA	A	672	46.572	-30.186	51.774	1.00	110.82	O
ATOM	4982	N	ALA	A	673	44.590	-31.233	52.047	1.00	112.36	N

379/396

Figure 3B-90

ATOM	4983	CA	ALA	A	673	44.983	-31.929	53.265	1.00	112.29	C
ATOM	4984	CB	ALA	A	673	43.994	-33.045	53.567	1.00	111.35	C
ATOM	4985	C	ALA	A	673	46.383	-32.500	53.105	1.00	112.67	C
ATOM	4986	O	ALA	A	673	47.192	-32.460	54.031	1.00	112.22	O
ATOM	4987	N	ALA	A	674	46.665	-33.025	51.919	1.00	112.98	N
ATOM	4988	CA	ALA	A	674	47.970	-33.602	51.635	1.00	113.76	C
ATOM	4989	CB	ALA	A	674	48.095	-33.896	50.153	1.00	114.05	C
ATOM	4990	C	ALA	A	674	49.084	-32.665	52.079	1.00	113.77	C
ATOM	4991	O	ALA	A	674	49.983	-33.063	52.817	1.00	113.98	O
ATOM	4992	N	ALA	A	675	49.021	-31.416	51.631	1.00	114.17	N
ATOM	4993	CA	ALA	A	675	50.037	-30.435	51.991	1.00	114.25	C
ATOM	4994	CB	ALA	A	675	50.061	-29.307	50.962	1.00	114.17	C
ATOM	4995	C	ALA	A	675	49.777	-29.874	53.383	1.00	113.66	C
ATOM	4996	O	ALA	A	675	50.703	-29.446	54.074	1.00	111.61	O
ATOM	4997	N	ALA	A	676	48.510	-29.887	53.788	1.00	114.84	N
ATOM	4998	CA	ALA	A	676	48.105	-29.382	55.098	1.00	116.66	C
ATOM	4999	CB	ALA	A	676	46.596	-29.140	55.116	1.00	117.13	C
ATOM	5000	C	ALA	A	676	48.499	-30.353	56.214	1.00	116.95	C
ATOM	5001	O	ALA	A	676	48.133	-30.171	57.381	1.00	116.44	O
ATOM	5002	N	ALA	A	677	49.245	-31.387	55.836	1.00	116.85	N
ATOM	5003	CA	ALA	A	677	49.718	-32.400	56.771	1.00	114.23	C
ATOM	5004	CB	ALA	A	677	48.964	-33.704	56.558	1.00	113.06	C
ATOM	5005	C	ALA	A	677	51.206	-32.607	56.524	1.00	112.65	C
ATOM	5006	O	ALA	A	677	51.615	-33.633	55.988	1.00	112.22	O
ATOM	5007	N	ALA	A	678	52.006	-31.617	56.903	1.00	110.96	N
ATOM	5008	CA	ALA	A	678	53.449	-31.687	56.727	1.00	110.69	C
ATOM	5009	CB	ALA	A	678	53.815	-31.315	55.307	1.00	108.59	C
ATOM	5010	C	ALA	A	678	54.145	-30.756	57.716	1.00	112.02	C
ATOM	5011	O	ALA	A	678	54.604	-29.671	57.343	1.00	110.40	O
ATOM	5012	N	ALA	A	679	54.215	-31.207	58.973	1.00	113.52	N
ATOM	5013	CA	ALA	A	679	54.830	-30.481	60.096	1.00	113.04	C
ATOM	5014	CB	ALA	A	679	55.883	-31.361	60.772	1.00	111.68	C
ATOM	5015	C	ALA	A	679	55.430	-29.117	59.758	1.00	112.78	C
ATOM	5016	O	ALA	A	679	56.651	-28.929	59.788	1.00	111.45	O
ATOM	5017	N	ALA	A	680	54.547	-28.171	59.447	1.00	112.51	N
ATOM	5018	CA	ALA	A	680	54.924	-26.805	59.111	1.00	113.14	C
ATOM	5019	CB	ALA	A	680	55.234	-26.697	57.613	1.00	113.58	C
ATOM	5020	C	ALA	A	680	53.761	-25.876	59.491	1.00	112.86	C
ATOM	5021	O	ALA	A	680	52.695	-26.399	59.889	1.00	111.63	O
ATOM	5022	OXT	ALA	A	680	53.925	-24.638	59.396	1.00	111.96	O
TER	5023		ALA	A	680					A	
ATOM	5024	CB	ALA	A	686	49.786	-23.562	61.895	1.00	103.53	C
ATOM	5025	C	ALA	A	686	50.555	-23.326	59.524	1.00	105.34	C
ATOM	5026	O	ALA	A	686	50.973	-22.161	59.474	1.00	106.05	O
ATOM	5027	N	ALA	A	686	52.089	-24.195	61.282	1.00	102.20	N
ATOM	5028	CA	ALA	A	686	50.678	-24.150	60.808	1.00	104.11	C
ATOM	5029	N	ALA	A	687	49.979	-23.942	58.491	1.00	104.90	N
ATOM	5030	CA	ALA	A	687	49.789	-23.296	57.191	1.00	102.36	C
ATOM	5031	CB	ALA	A	687	51.036	-23.497	56.313	1.00	101.16	C
ATOM	5032	C	ALA	A	687	48.549	-23.849	56.482	1.00	100.09	C
ATOM	5033	O	ALA	A	687	48.648	-24.542	55.469	1.00	100.04	O
ATOM	5034	N	ALA	A	688	47.380	-23.532	57.026	1.00	97.10	N
ATOM	5035	CA	ALA	A	688	46.121	-23.986	56.457	1.00	94.50	C
ATOM	5036	CB	ALA	A	688	44.958	-23.323	57.186	1.00	92.48	C
ATOM	5037	C	ALA	A	688	46.029	-23.703	54.959	1.00	92.73	C
ATOM	5038	O	ALA	A	688	45.668	-22.600	54.546	1.00	91.75	O

380/396

Figure 3B-91

ATOM	5039	N	ALA	A	689	46.368	-24.702	54.151	1.00	91.41	N
ATOM	5040	CA	ALA	A	689	46.293	-24.584	52.697	1.00	90.98	C
ATOM	5041	CB	ALA	A	689	47.544	-25.165	52.052	1.00	87.28	C
ATOM	5042	C	ALA	A	689	45.069	-25.394	52.292	1.00	91.63	C
ATOM	5043	O	ALA	A	689	44.957	-26.558	52.671	1.00	92.18	O
ATOM	5044	N	ALA	A	690	44.147	-24.794	51.540	1.00	92.69	N
ATOM	5045	CA	ALA	A	690	42.939	-25.516	51.135	1.00	93.72	C
ATOM	5046	CB	ALA	A	690	41.848	-25.325	52.189	1.00	93.60	C
ATOM	5047	C	ALA	A	690	42.392	-25.165	49.747	1.00	93.34	C
ATOM	5048	O	ALA	A	690	42.814	-24.187	49.135	1.00	92.06	O
ATOM	5049	N	ALA	A	691	41.448	-25.987	49.279	1.00	94.80	N
ATOM	5050	CA	ALA	A	691	40.797	-25.852	47.969	1.00	95.39	C
ATOM	5051	CB	ALA	A	691	39.422	-26.514	47.988	1.00	93.22	C
ATOM	5052	C	ALA	A	691	40.655	-24.417	47.521	1.00	96.50	C
ATOM	5053	O	ALA	A	691	39.569	-23.840	47.596	1.00	98.44	O
ATOM	5054	N	ALA	A	692	41.759	-23.861	47.035	1.00	95.84	N
ATOM	5055	CA	ALA	A	692	41.812	-22.488	46.565	1.00	94.27	C
ATOM	5056	CB	ALA	A	692	41.259	-21.544	47.625	1.00	92.42	C
ATOM	5057	C	ALA	A	692	43.272	-22.173	46.299	1.00	94.25	C
ATOM	5058	O	ALA	A	692	43.600	-21.152	45.703	1.00	95.63	O
ATOM	5059	N	ALA	A	693	44.150	-23.064	46.742	1.00	94.08	N
ATOM	5060	CA	ALA	A	693	45.580	-22.867	46.557	1.00	94.67	C
ATOM	5061	CB	ALA	A	693	46.308	-23.137	47.864	1.00	94.38	C
ATOM	5062	C	ALA	A	693	46.138	-23.751	45.446	1.00	95.35	C
ATOM	5063	O	ALA	A	693	47.354	-23.786	45.223	1.00	94.67	O
ATOM	5064	N	ALA	A	694	45.242	-24.454	44.752	1.00	95.62	N
ATOM	5065	CA	ALA	A	694	45.620	-25.346	43.658	1.00	96.30	C
ATOM	5066	CB	ALA	A	694	44.675	-26.534	43.618	1.00	93.34	C
ATOM	5067	C	ALA	A	694	45.621	-24.624	42.303	1.00	98.59	C
ATOM	5068	O	ALA	A	694	45.974	-23.443	42.214	1.00	98.78	O
ATOM	5069	N	ALA	A	695	45.229	-25.337	41.249	1.00	99.79	N
ATOM	5070	CA	ALA	A	695	45.189	-24.757	39.908	1.00	99.98	C
ATOM	5071	CB	ALA	A	695	46.550	-24.155	39.555	1.00	99.29	C
ATOM	5072	C	ALA	A	695	44.803	-25.810	38.878	1.00	100.09	C
ATOM	5073	O	ALA	A	695	45.652	-26.295	38.138	1.00	99.80	O
ATOM	5074	N	ALA	A	696	43.519	-26.148	38.827	1.00	100.85	N
ATOM	5075	CA	ALA	A	696	43.020	-27.158	37.895	1.00	102.87	C
ATOM	5076	CB	ALA	A	696	41.555	-27.465	38.205	1.00	100.34	C
ATOM	5077	C	ALA	A	696	43.171	-26.791	36.414	1.00	104.45	C
ATOM	5078	O	ALA	A	696	42.254	-26.227	35.817	1.00	104.75	O
ATOM	5079	N	ALA	A	697	44.322	-27.124	35.826	1.00	105.93	N
ATOM	5080	CA	ALA	A	697	44.586	-26.843	34.410	1.00	106.86	C
ATOM	5081	CB	ALA	A	697	46.084	-26.671	34.167	1.00	106.75	C
ATOM	5082	C	ALA	A	697	44.048	-27.978	33.546	1.00	107.20	C
ATOM	5083	O	ALA	A	697	43.238	-28.776	34.017	1.00	105.67	O
ATOM	5084	N	ALA	A	698	44.506	-28.052	32.295	1.00	108.10	N
ATOM	5085	CA	ALA	A	698	44.053	-29.088	31.369	1.00	108.56	C
ATOM	5086	CB	ALA	A	698	44.903	-30.342	31.529	1.00	108.91	C
ATOM	5087	C	ALA	A	698	42.581	-29.403	31.642	1.00	109.13	C
ATOM	5088	O	ALA	A	698	41.695	-28.716	31.142	1.00	109.63	O
ATOM	5089	N	ALA	A	699	42.335	-30.436	32.444	1.00	110.42	N
ATOM	5090	CA	ALA	A	699	40.984	-30.867	32.838	1.00	111.86	C
ATOM	5091	CB	ALA	A	699	40.629	-30.277	34.210	1.00	110.75	C
ATOM	5092	C	ALA	A	699	39.857	-30.576	31.849	1.00	111.87	C
ATOM	5093	O	ALA	A	699	38.908	-29.855	32.230	1.00	110.52	O
ATOM	5094	OXT	ALA	A	699	39.928	-31.088	30.713	1.00	113.27	O

381/396

Figure 3B-92

TER	5095		ALA	A	699				A	
ATOM	5096	CB	ALA	A	701	35.443	-44.027	35.083	1.00	113.62 C
ATOM	5097	C	ALA	A	701	37.903	-44.094	34.655	1.00	117.34 C
ATOM	5098	O	ALA	A	701	38.210	-42.900	34.676	1.00	117.51 O
ATOM	5099	N	ALA	A	701	36.466	-46.018	34.030	1.00	113.60 N
ATOM	5100	CA	ALA	A	701	36.534	-44.532	34.144	1.00	115.79 C
ATOM	5101	N	ALA	A	702	38.713	-45.072	35.064	1.00	118.80 N
ATOM	5102	CA	ALA	A	702	40.064	-44.837	35.583	1.00	119.25 C
ATOM	5103	CB	ALA	A	702	41.068	-44.771	34.425	1.00	117.28 C
ATOM	5104	C	ALA	A	702	40.177	-43.578	36.444	1.00	119.85 C
ATOM	5105	O	ALA	A	702	39.387	-43.375	37.370	1.00	119.84 O
ATOM	5106	N	ALA	A	703	41.171	-42.748	36.127	1.00	119.79 N
ATOM	5107	CA	ALA	A	703	41.434	-41.496	36.838	1.00	118.82 C
ATOM	5108	CB	ALA	A	703	41.453	-41.732	38.342	1.00	118.45 C
ATOM	5109	C	ALA	A	703	42.781	-40.949	36.386	1.00	118.73 C
ATOM	5110	O	ALA	A	703	42.873	-39.812	35.925	1.00	116.96 O
ATOM	5111	N	ALA	A	704	43.811	-41.782	36.532	1.00	120.17 N
ATOM	5112	CA	ALA	A	704	45.195	-41.467	36.161	1.00	120.78 C
ATOM	5113	CB	ALA	A	704	45.231	-40.429	35.029	1.00	120.25 C
ATOM	5114	C	ALA	A	704	46.029	-40.976	37.347	1.00	120.41 C
ATOM	5115	O	ALA	A	704	46.858	-40.077	37.198	1.00	120.35 O
ATOM	5116	N	ALA	A	705	45.818	-41.579	38.516	1.00	119.56 N
ATOM	5117	CA	ALA	A	705	46.547	-41.193	39.722	1.00	118.18 C
ATOM	5118	CB	ALA	A	705	46.267	-42.188	40.843	1.00	115.36 C
ATOM	5119	C	ALA	A	705	48.042	-41.129	39.450	1.00	118.17 C
ATOM	5120	O	ALA	A	705	48.542	-40.034	39.111	1.00	118.44 O
ATOM	5121	OXT	ALA	A	705	48.692	-42.186	39.563	1.00	119.24 O
TER	5122		ALA	A	705				A	
ATOM	5123	CB	ALA	A	804	47.903	-28.623	39.856	1.00	95.79 C
ATOM	5124	C	ALA	A	804	49.540	-27.029	40.866	1.00	99.63 C
ATOM	5125	O	ALA	A	804	50.478	-27.773	40.574	1.00	98.69 O
ATOM	5126	N	ALA	A	804	48.188	-26.348	38.917	1.00	98.49 N
ATOM	5127	CA	ALA	A	804	48.194	-27.156	40.169	1.00	98.70 C
ATOM	5128	N	ALA	A	805	49.624	-26.068	41.781	1.00	100.87 N
ATOM	5129	CA	ALA	A	805	50.836	-25.819	42.552	1.00	102.12 C
ATOM	5130	CB	ALA	A	805	51.649	-24.692	41.915	1.00	102.13 C
ATOM	5131	C	ALA	A	805	50.436	-25.455	43.985	1.00	102.86 C
ATOM	5132	O	ALA	A	805	49.294	-25.686	44.384	1.00	101.82 O
ATOM	5133	N	ALA	A	806	51.361	-24.877	44.749	1.00	104.12 N
ATOM	5134	CA	ALA	A	806	51.083	-24.522	46.144	1.00	104.86 C
ATOM	5135	CB	ALA	A	806	52.123	-25.174	47.057	1.00	104.21 C
ATOM	5136	C	ALA	A	806	51.010	-23.024	46.441	1.00	103.98 C
ATOM	5137	O	ALA	A	806	51.047	-22.198	45.528	1.00	103.67 O
ATOM	5138	N	ALA	A	807	50.900	-22.714	47.736	1.00	103.05 N
ATOM	5139	CA	ALA	A	807	50.819	-21.353	48.286	1.00	102.62 C
ATOM	5140	CB	ALA	A	807	51.358	-20.323	47.294	1.00	104.70 C
ATOM	5141	C	ALA	A	807	49.412	-20.963	48.706	1.00	101.03 C
ATOM	5142	O	ALA	A	807	48.449	-21.206	47.985	1.00	100.71 O
ATOM	5143	N	ALA	A	808	49.304	-20.354	49.881	1.00	100.36 N
ATOM	5144	CA	ALA	A	808	48.017	-19.902	50.403	1.00	100.82 C
ATOM	5145	CB	ALA	A	808	47.465	-20.910	51.406	1.00	99.74 C
ATOM	5146	C	ALA	A	808	48.210	-18.544	51.072	1.00	100.65 C
ATOM	5147	O	ALA	A	808	49.109	-18.377	51.898	1.00	100.39 O
ATOM	5148	N	ALA	A	809	47.369	-17.581	50.700	1.00	99.77 N
ATOM	5149	CA	ALA	A	809	47.422	-16.220	51.237	1.00	99.44 C
ATOM	5150	CB	ALA	A	809	47.592	-16.253	52.762	1.00	98.70 C

382/396

Figure 3B-93

ATOM	5151	C	ALA	A	809	48.530	-15.378	50.588	1.00	98.87	C
ATOM	5152	O	ALA	A	809	48.936	-14.342	51.112	1.00	98.96	O
ATOM	5153	N	ALA	A	810	49.006	-15.834	49.437	1.00	99.08	N
ATOM	5154	CA	ALA	A	810	50.043	-15.145	48.674	1.00	100.56	C
ATOM	5155	CB	ALA	A	810	51.310	-14.986	49.503	1.00	100.00	C
ATOM	5156	C	ALA	A	810	50.318	-15.996	47.442	1.00	102.50	C
ATOM	5157	O	ALA	A	810	51.432	-16.488	47.250	1.00	102.69	O
ATOM	5158	N	ALA	A	811	49.278	-16.171	46.624	1.00	104.18	N
ATOM	5159	CA	ALA	A	811	49.340	-16.963	45.399	1.00	105.11	C
ATOM	5160	CB	ALA	A	811	47.988	-16.955	44.709	1.00	104.33	C
ATOM	5161	C	ALA	A	811	50.415	-16.478	44.439	1.00	106.43	C
ATOM	5162	O	ALA	A	811	50.289	-16.633	43.224	1.00	103.83	O
ATOM	5163	N	ALA	A	812	51.465	-15.882	44.997	1.00	109.58	N
ATOM	5164	CA	ALA	A	812	52.594	-15.390	44.225	1.00	111.96	C
ATOM	5165	CB	ALA	A	812	53.469	-14.481	45.091	1.00	110.97	C
ATOM	5166	C	ALA	A	812	53.370	-16.631	43.802	1.00	114.10	C
ATOM	5167	O	ALA	A	812	54.582	-16.579	43.580	1.00	114.98	O
ATOM	5168	N	ALA	A	813	52.641	-17.745	43.719	1.00	116.14	N
ATOM	5169	CA	ALA	A	813	53.167	-19.052	43.330	1.00	117.72	C
ATOM	5170	CB	ALA	A	813	54.261	-18.894	42.273	1.00	117.67	C
ATOM	5171	C	ALA	A	813	53.692	-19.872	44.509	1.00	118.83	C
ATOM	5172	O	ALA	A	813	53.806	-19.371	45.630	1.00	119.00	O
ATOM	5173	N	ALA	A	814	53.999	-21.137	44.224	1.00	119.17	N
ATOM	5174	CA	ALA	A	814	54.523	-22.100	45.190	1.00	118.98	C
ATOM	5175	CB	ALA	A	814	54.099	-21.740	46.609	1.00	118.55	C
ATOM	5176	C	ALA	A	814	54.010	-23.491	44.832	1.00	118.52	C
ATOM	5177	O	ALA	A	814	54.361	-24.042	43.789	1.00	118.08	O
ATOM	5178	N	ALA	A	816	55.118	-25.432	46.906	1.00	113.08	N
ATOM	5179	CA	ALA	A	816	56.283	-25.156	46.077	1.00	114.83	C
ATOM	5180	CB	ALA	A	816	57.369	-24.493	46.913	1.00	113.21	C
ATOM	5181	C	ALA	A	816	56.814	-26.437	45.436	1.00	116.46	C
ATOM	5182	O	ALA	A	816	56.041	-27.314	45.049	1.00	116.95	O
ATOM	5183	N	ALA	A	817	58.134	-26.540	45.328	1.00	117.42	N
ATOM	5184	CA	ALA	A	817	58.764	-27.710	44.728	1.00	118.82	C
ATOM	5185	CB	ALA	A	817	60.231	-27.417	44.451	1.00	118.05	C
ATOM	5186	C	ALA	A	817	58.632	-28.947	45.619	1.00	120.39	C
ATOM	5187	O	ALA	A	817	58.298	-28.837	46.800	1.00	121.02	O
ATOM	5188	N	ALA	A	818	58.897	-30.118	45.039	1.00	121.34	N
ATOM	5189	CA	ALA	A	818	58.826	-31.401	45.747	1.00	120.72	C
ATOM	5190	CB	ALA	A	818	59.857	-31.436	46.870	1.00	121.00	C
ATOM	5191	C	ALA	A	818	57.436	-31.709	46.303	1.00	120.75	C
ATOM	5192	O	ALA	A	818	57.277	-32.593	47.148	1.00	118.92	O
ATOM	5193	N	ALA	A	819	56.434	-30.980	45.817	1.00	121.40	N
ATOM	5194	CA	ALA	A	819	55.051	-31.167	46.247	1.00	120.14	C
ATOM	5195	CB	ALA	A	819	54.122	-30.307	45.402	1.00	119.98	C
ATOM	5196	C	ALA	A	819	54.670	-32.633	46.112	1.00	119.34	C
ATOM	5197	O	ALA	A	819	53.601	-33.055	46.561	1.00	117.60	O
ATOM	5198	N	ALA	A	820	55.551	-33.397	45.471	1.00	119.08	N
ATOM	5199	CA	ALA	A	820	55.340	-34.822	45.283	1.00	118.48	C
ATOM	5200	CB	ALA	A	820	56.597	-35.464	44.713	1.00	117.18	C
ATOM	5201	C	ALA	A	820	55.026	-35.399	46.655	1.00	118.23	C
ATOM	5202	O	ALA	A	820	53.982	-36.025	46.857	1.00	118.92	O
ATOM	5203	N	ALA	A	821	55.938	-35.155	47.593	1.00	116.15	N
ATOM	5204	CA	ALA	A	821	55.813	-35.616	48.971	1.00	114.17	C
ATOM	5205	CB	ALA	A	821	55.983	-34.437	49.926	1.00	114.83	C
ATOM	5206	C	ALA	A	821	54.499	-36.331	49.261	1.00	112.36	C

383/396

Figure 3B-94

ATOM	5207	O	ALA	A	821	54.351	-37.513	48.958	1.00	112.55	O
ATOM	5208	N	ALA	A	822	53.550	-35.602	49.842	1.00	110.48	N
ATOM	5209	CA	ALA	A	822	52.244	-36.149	50.202	1.00	110.19	C
ATOM	5210	CB	ALA	A	822	51.186	-35.060	50.121	1.00	109.83	C
ATOM	5211	C	ALA	A	822	51.820	-37.349	49.363	1.00	110.04	C
ATOM	5212	O	ALA	A	822	51.972	-37.355	48.138	1.00	109.40	O
ATOM	5213	N	ALA	A	823	51.286	-38.366	50.036	1.00	110.07	N
ATOM	5214	CA	ALA	A	823	50.839	-39.580	49.367	1.00	109.54	C
ATOM	5215	CB	ALA	A	823	52.011	-40.538	49.200	1.00	109.28	C
ATOM	5216	C	ALA	A	823	49.707	-40.266	50.129	1.00	109.33	C
ATOM	5217	O	ALA	A	823	49.496	-40.007	51.316	1.00	107.65	O
ATOM	5218	N	ALA	A	824	48.984	-41.133	49.421	1.00	110.38	N
ATOM	5219	CA	ALA	A	824	47.865	-41.902	49.969	1.00	112.00	C
ATOM	5220	CB	ALA	A	824	48.269	-42.546	51.296	1.00	111.45	C
ATOM	5221	C	ALA	A	824	46.578	-41.096	50.150	1.00	112.98	C
ATOM	5222	O	ALA	A	824	46.589	-40.011	50.730	1.00	113.33	O
ATOM	5223	N	ALA	A	825	45.470	-41.645	49.654	1.00	113.29	N
ATOM	5224	CA	ALA	A	825	44.166	-40.993	49.754	1.00	112.89	C
ATOM	5225	CB	ALA	A	825	43.997	-39.994	48.617	1.00	112.06	C
ATOM	5226	C	ALA	A	825	43.018	-42.010	49.739	1.00	113.03	C
ATOM	5227	O	ALA	A	825	42.335	-42.129	48.697	1.00	112.10	O
ATOM	5228	OXT	ALA	A	825	42.818	-42.688	50.771	1.00	112.07	O
TER	5229		ALA	A	825					A	
ATOM	5230	OH2	TIP		1	43.985	32.160	23.687	1.00	50.16	O
ATOM	5231	OH2	TIP		2	46.122	7.949	20.002	1.00	44.36	O
ATOM	5232	OH2	TIP		3	30.079	-10.774	16.015	1.00	42.09	O
ATOM	5233	OH2	TIP		4	64.801	7.121	25.195	1.00	50.58	O
ATOM	5234	OH2	TIP		5	34.333	8.797	22.364	1.00	49.06	O
ATOM	5235	OH2	TIP		6	44.405	2.935	45.111	1.00	53.58	O
ATOM	5236	OH2	TIP		7	30.891	-5.705	25.883	1.00	47.61	O
ATOM	5237	OH2	TIP		8	38.688	28.090	8.194	1.00	53.52	O
ATOM	5238	OH2	TIP		9	68.042	-2.318	28.253	1.00	71.02	O
ATOM	5239	OH2	TIP		10	57.832	13.375	2.921	1.00	70.13	O
ATOM	5240	OH2	TIP		11	42.091	-9.023	48.235	1.00	74.47	O
ATOM	5241	OH2	TIP		12	43.335	-0.744	22.234	1.00	56.11	O
ATOM	5242	OH2	TIP		13	31.462	9.289	27.481	1.00	50.36	O
ATOM	5243	OH2	TIP		14	18.234	26.825	5.609	1.00	63.03	O
ATOM	5244	OH2	TIP		15	20.463	-0.151	19.908	1.00	70.45	O
TER	5245		TIP		15					S	
ATOM	5246	C1	NAG	N	800	18.060	19.760	1.829	1.00	126.15	C
ATOM	5247	C2	NAG	N	800	19.242	20.685	2.267	1.00	124.16	C
ATOM	5248	N2	NAG	N	800	20.522	20.072	1.959	1.00	125.23	N
ATOM	5249	C7	NAG	N	800	21.501	20.806	1.429	1.00	126.58	C
ATOM	5250	O7	NAG	N	800	21.638	20.937	0.213	1.00	129.33	O
ATOM	5251	C8	NAG	N	800	22.468	21.515	2.376	1.00	123.82	C
ATOM	5252	C3	NAG	N	800	19.207	21.101	3.749	1.00	122.13	C
ATOM	5253	O3	NAG	N	800	20.074	22.202	3.944	1.00	123.01	O
ATOM	5254	C4	NAG	N	800	17.802	21.507	4.136	1.00	120.45	C
ATOM	5255	O4	NAG	N	800	17.737	21.888	5.500	1.00	120.92	O
ATOM	5256	C5	NAG	N	800	16.881	20.344	3.866	1.00	121.66	C
ATOM	5257	O5	NAG	N	800	16.795	20.148	2.435	1.00	124.47	O
ATOM	5258	C6	NAG	N	800	15.486	20.604	4.412	1.00	122.53	C
ATOM	5259	O6	NAG	N	800	14.709	21.393	3.527	1.00	124.52	O
ATOM	5260	C1	NAG	N	801	9.344	-0.202	15.773	1.00	118.09	C
ATOM	5261	C2	NAG	N	801	9.341	-0.470	14.265	1.00	118.54	C
ATOM	5262	N2	NAG	N	801	9.808	0.688	13.528	1.00	121.14	N

Figure 3B-95

ATOM	5263	C7	NAG	N	801	10.388	0.512	12.343	1.00	121.75	C
ATOM	5264	O7	NAG	N	801	11.078	-0.477	12.088	1.00	122.37	O
ATOM	5265	C8	NAG	N	801	10.144	1.562	11.263	1.00	120.95	C
ATOM	5266	C3	NAG	N	801	7.918	-0.863	13.832	1.00	117.05	C
ATOM	5267	O3	NAG	N	801	7.905	-1.188	12.450	1.00	116.34	O
ATOM	5268	C4	NAG	N	801	7.437	-2.074	14.653	1.00	115.54	C
ATOM	5269	O4	NAG	N	801	6.061	-2.324	14.390	1.00	114.08	O
ATOM	5270	C5	NAG	N	801	7.648	-1.850	16.178	1.00	115.71	C
ATOM	5271	O5	NAG	N	801	9.012	-1.413	16.465	1.00	118.26	O
ATOM	5272	C6	NAG	N	801	7.436	-3.131	16.958	1.00	112.74	C
ATOM	5273	O6	NAG	N	801	8.678	-3.731	17.304	1.00	109.75	O
TER	5274		NAG	N	801					N	
ATOM	5275	O1	XX5	Z	500	38.645	6.536	23.562	1.00	29.75	O
ATOM	5276	C2	XX5	Z	500	38.337	6.940	24.663	1.00	34.41	C
ATOM	5277	O3	XX5	Z	500	37.964	8.094	24.829	1.00	32.96	O
ATOM	5278	C4	XX5	Z	500	38.445	5.962	25.861	1.00	40.37	C
ATOM	5279	C5	XX5	Z	500	37.148	5.634	26.620	1.00	40.53	C
ATOM	5280	C6	XX5	Z	500	35.809	6.179	26.159	1.00	40.80	C
ATOM	5281	C7	XX5	Z	500	34.768	5.749	27.171	1.00	47.75	C
ATOM	5282	C8	XX5	Z	500	35.411	5.576	24.803	1.00	45.40	C
ATOM	5283	N9	XX5	Z	500	39.453	6.362	26.844	1.00	46.45	N
ATOM	5284	C10	XX5	Z	500	40.825	6.002	26.475	1.00	49.51	C
ATOM	5285	C11	XX5	Z	500	41.055	4.500	26.115	1.00	48.11	C
ATOM	5286	O12	XX5	Z	500	41.375	4.225	24.961	1.00	45.92	O
ATOM	5287	O13	XX5	Z	500	40.927	3.643	26.978	1.00	47.76	O
ATOM	5288	C14	XX5	Z	500	41.821	6.437	27.579	1.00	48.29	C
ATOM	5289	C15	XX5	Z	500	43.230	6.191	27.086	1.00	46.79	C
ATOM	5290	C16	XX5	Z	500	43.811	6.821	25.973	1.00	42.21	C
ATOM	5291	N17	XX5	Z	500	45.047	6.337	25.862	1.00	50.64	N
ATOM	5292	C18	XX5	Z	500	45.205	5.450	26.871	1.00	48.30	C
ATOM	5293	N19	XX5	Z	500	44.138	5.307	27.666	1.00	45.77	N
ATOM	5294	C20	XX5	Z	500	43.945	4.421	28.889	1.00	44.21	C
ATOM	5295	C21	XX5	Z	500	44.054	5.110	30.261	1.00	44.11	C
ATOM	5296	C22	XX5	Z	500	44.875	6.260	30.331	1.00	46.80	C
ATOM	5297	C23	XX5	Z	500	45.048	6.985	31.517	1.00	52.98	C
ATOM	5298	CL24	XX5	Z	500	46.098	8.414	31.495	1.00	56.82	CL
ATOM	5299	C25	XX5	Z	500	44.390	6.582	32.724	1.00	46.90	C
ATOM	5300	C26	XX5	Z	500	43.385	4.689	31.470	1.00	41.08	C
ATOM	5301	C27	XX5	Z	500	43.554	5.434	32.712	1.00	46.71	C
ATOM	5302	CL28	XX5	Z	500	42.727	4.946	34.238	1.00	40.50	CL
TER	5303		XX5	Z	500					Z	
ATOM	5304	ZN	ZN	T	1	39.163	8.159	22.508	1.00	39.19	ZN
TER	5305		ZN	T	1						
ATOM	5306	CL	CL	C	999	43.173	-10.945	30.569	1.00	58.44	CL
TER	5307		CL	C	999					C	
END											

385/396

Figure 4

		$\alpha 1$		$\alpha 2$		
ACE2	19	STIEEQAKTFLDKFNHEAEDLFYQSSLASWNYNTNITEENVQNMNAGDKWSAFLKEQST	78			
sACE	614	VTDEAEASKFVEEYDRTSQVWVNEYAEANWNYNTNITTETSKILLQKNMQIANHTLK YGT	673			
tACE	38	VTDEAEASKFVEEYDRTSQVWVNEYAEANWNYNTNITTETSKILLQKNMQIANHTLK YGT	97			
		* * * *	* * * * * *		*	
		$\alpha 3$		$\alpha 4$	$\beta 1$	
ACE2	79	LAQMYPLQEIQNLT VKLQ LQALQQNGSSVLSSEDKSKRLNTILNTMSTIYSTGKVCNPDNP	138			
sACE	674	QARKFDVNQLQNTTIKRI IKKVQDLERAALPAQELEEYNKILLDMETTYSVATVCHPNG-	732			
tACE	98	QARKFDVNQLQNTTIKRI IKKVQDLERAALPAQELEEYNKILLDMETTYSVATVCHPNG-	156			
		* * * *	* * * * *	* * *		
		$\beta 2$	$\alpha 5$	$\alpha 6$		
ACE2	139	QECLLLEPGLNEIMANSLDYNERLWAWESWRSEVGKQLRPLYEEYVVLKNEMARANHYED	198			
sACE	733	-SCLQLEPDLTNVMATSRKYEDLLWAWEGWRDKAGRAILQFYPKYVELINQAARLNGYVD	791			
tACE	157	-SCLQLEPDLTNVMATSRKYEDLLWAWEGWRDKAGRAILQFYPKYVELINQAARLNGYVD	215			
		** * * *	* * * * *	* * * * *	* * *	
		$\alpha 7$		$\alpha 8$		
ACE2	199	YGDYWRGDYEVNGVDGYDYSRGLIEDVEHTFEEIKPLYEHLHAYVRAKL MNAY-PSYIS	257			
sACE	792	AGDSWRSMYETP-----SLEQDLERLFQELQPLYLNLHAYVRRALHRRHYGAQHIN	841			
tACE	216	AGDSWRSMYETP-----SLEQDLERLFQELQPLYLNLHAYVRRALHRRHYGAQHIN	265			
		* * *	* * * * *	* * * * *	* *	
		$\beta 3$	$\alpha 9$	$\alpha 10$	$\alpha 11$	
ACE2	258	PIGCLP-AHLLGDMWGRFWTNLYSLTVPFGQKPNIDVTDAMVDQAWDAQRI FKEAEKFFV	317			
sACE	842	LEGPIP-AHLLGNMWAQTWSNIYDLVVPFPSPAPSMDTTEAMLKQGWTPRRMFKEADDDFT	900			
tACE	266	LEGPIP-AHLLGNMWAQTWSNIYDLVVPFPSPAPSMDTTEAMLKQGWTPRRMFKEADDDFT	324			
		* * * * *	* * * * *	* * * * *	* * *	
		$\alpha 12$	$\beta 4$	$\beta 5$	$\beta 6$	$\alpha 13$
ACE2	318	SVGLPNMTQGFWENSMLTDPGNVQKAVCHPTAWDLGKG-DFRILMCTKV TMDDFLT AHHE	375			
sACE	901	SLGLLPVPPEFWNKSMLKPTDGREVVCHASAWDFYNGKDFRIKQCTTVNLEDLVVAHHE	960			
tACE	325	SLGLLPVPPEFWNKSMLKPTDGREVVCHASAWDFYNGKDFRIKQCTTVNLEDLVVAHHE	384			
		* *	* * *	* * *	* * *	* * *
		$\alpha 13$		$\alpha 14$	$\alpha 15$	
ACE2	376	MGHIQYDMAYAAQPFLLRNGAN--EGFHEAVGEIMSLSAATPKHLKSI GLLSPDFQEDNE	433			
sACE	961	MGHIQYFMQYKDL PVALREGAN--PGFHEAIGDVLALS SVSTPKHLHSLNLLSSEGGSD-E	1017			
tACE	385	MGHIQYFMQYKDL PVALREGAN--PGFHEAIGDVLALS SVSTPKHLHSLNLLSSEGGSD-E	441			
		* * * * *	* * * * *	* * * * *	* * *	*
		$\alpha 16$	$\alpha 17$	$\alpha 18$	$\beta 7$	
ACE2	434	TEINFL LKQALTIVGTL PFTYMLEKWRWMVFKGEIPKDQWMKKWEMKREIVGVPEPVPH	493			
sACE	1018	HDINFLMKMALDKIAFI PFSYLVDQWRWRVFDGSITKENYNQEWWSLRLKYQGLCPPVPR	1077			
tACE	442	HDINFLMKMALDKIAFI PFSYLVDQWRWRVFDGSITKENYNQEWWSLRLKYQGLCPPVPR	501			
		* * *	* * *	* * *	* * *	
		$\alpha 19$	$\alpha 20$	$\alpha 21$		
ACE2	494	DETYCDPASLFHVSNDYSFIRYTRTYLQFQFQEALCQA AKHEGPLHKCDISNSTEAGQK	553			
sACE	1078	TQGD FDPGAKFHIPSSVPYIRYFVSFIIQFQFHEALCQAAGHTGPLHKCDIYQSKEAGQR	1137			
tACE	502	TQGD FDPGAKFHIPSSVPYIRYFVSFIIQFQFHEALCQAAGHTGPLHKCDIYQSKEAGQR	561			
		** *	* * *	* * * * *	* * *	
		$\alpha 22$	$\alpha 23$			▼
ACE2	554	LFN-MLRLGKSEPWT LALENVVGA-KNMNVRPLLNYFEPLFTWLKDQNK--NSFVGW-STDWSPY	613			
sACE	1138	LAT-AMKLGFSRFPWEAMQLITGQ-PNMSASAMLSYFKPLLDWLRTENELHGEKLGWPQYNWTPN	1200			
tACE	562	LAT-AMKLGFSRFPWEAMQLITGQ-PNMSASAMLSYFKPLLDWLRTENELHGEKLGWPQYNWTPN	624			
		*	* * * * *	* * *	* *	

Figure 5A

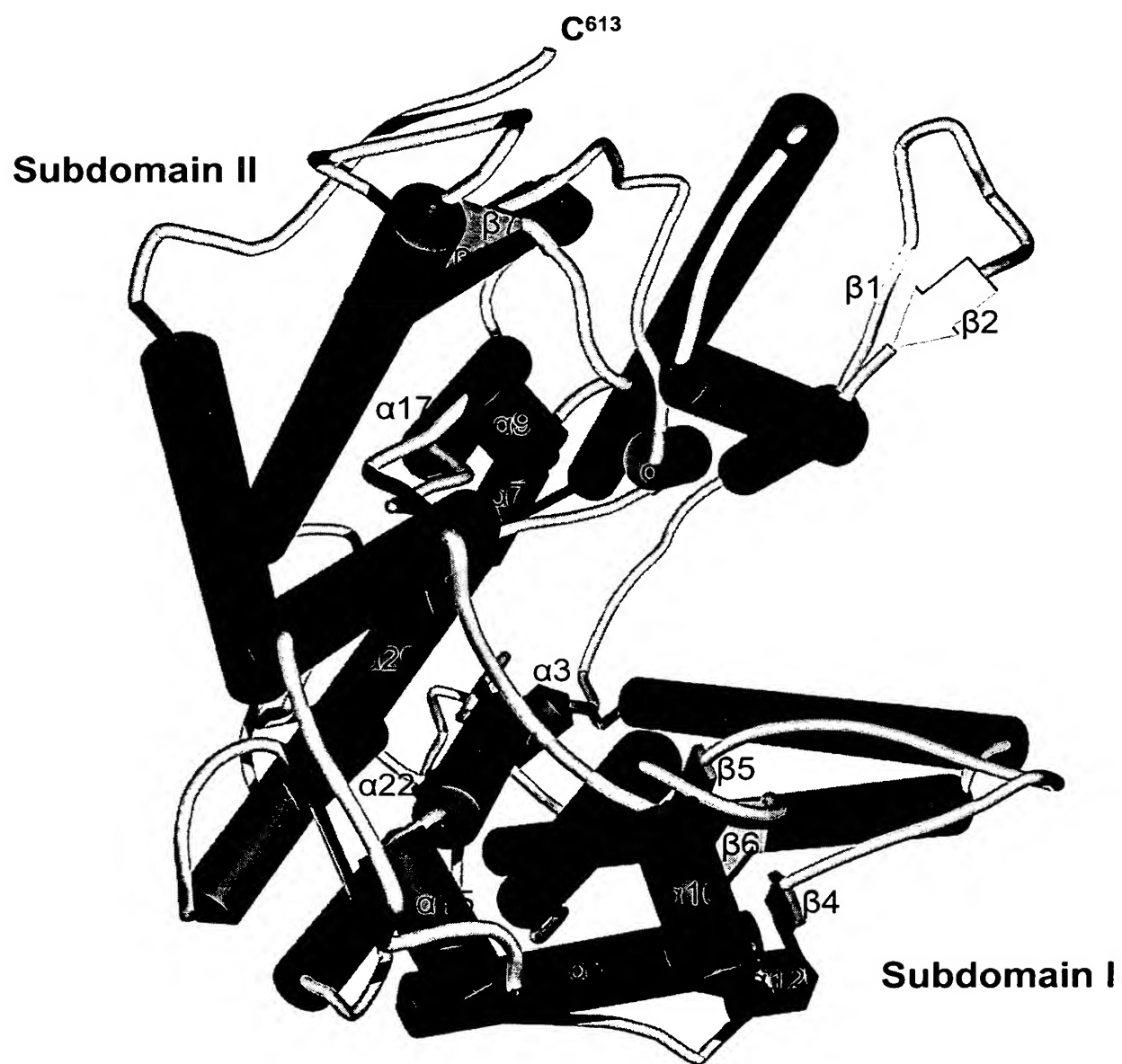


Figure 5B

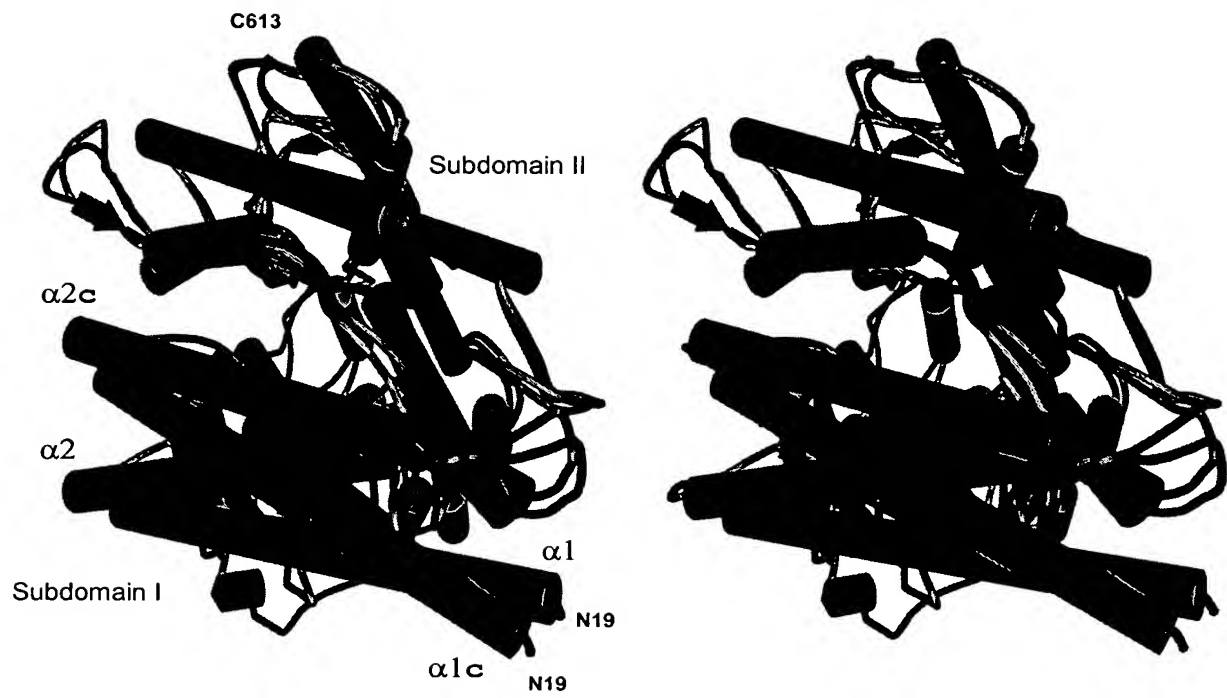
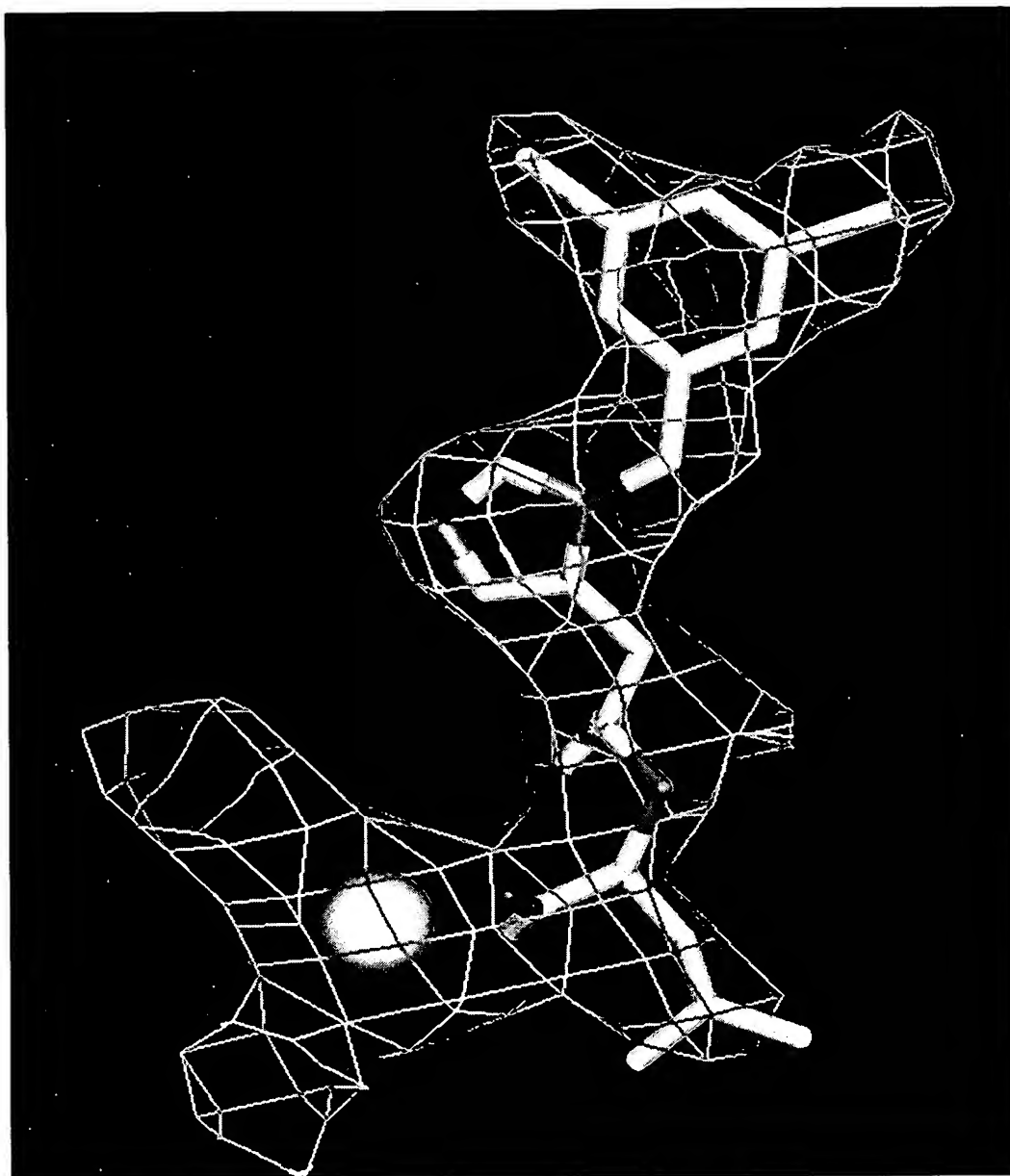


Figure 6



389/396

Figure 7



390/396

Figure 8A

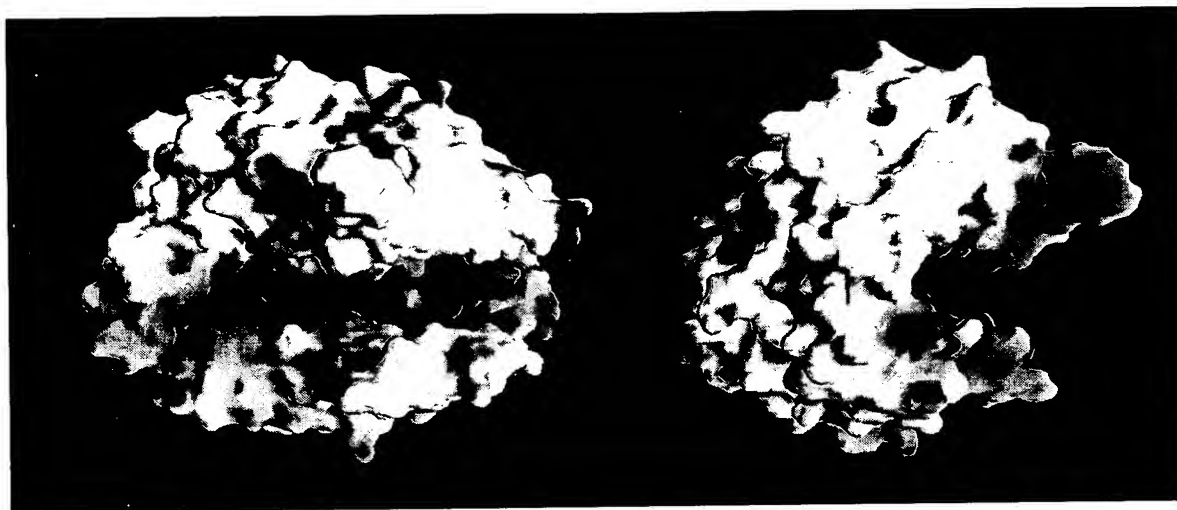
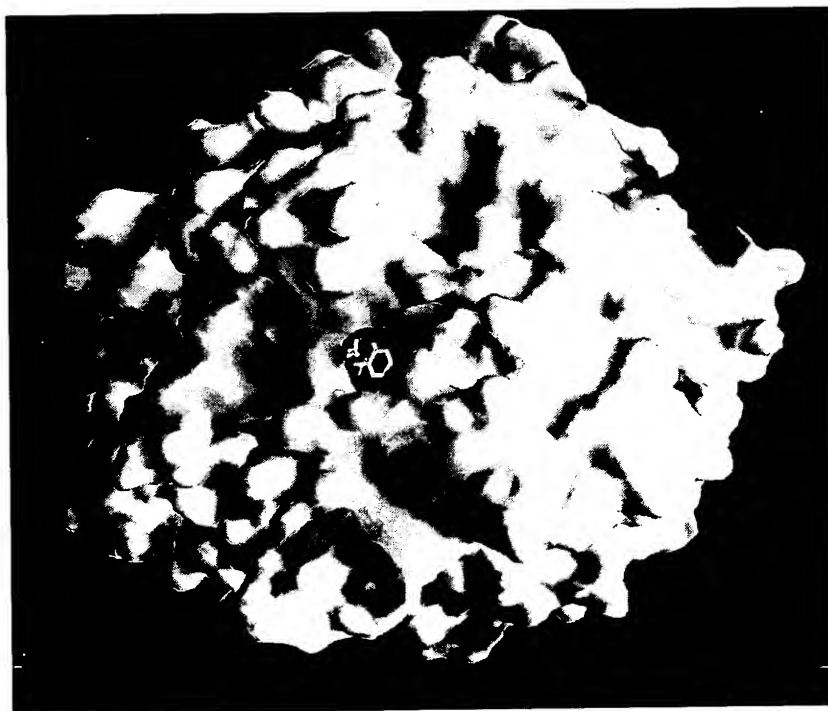


Figure 8B



391/396

Figure 9A

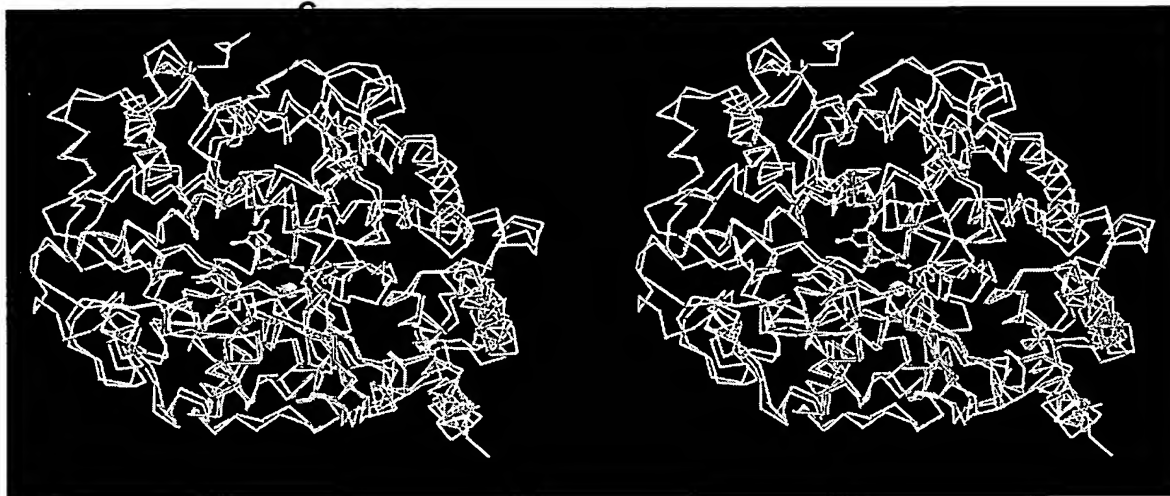
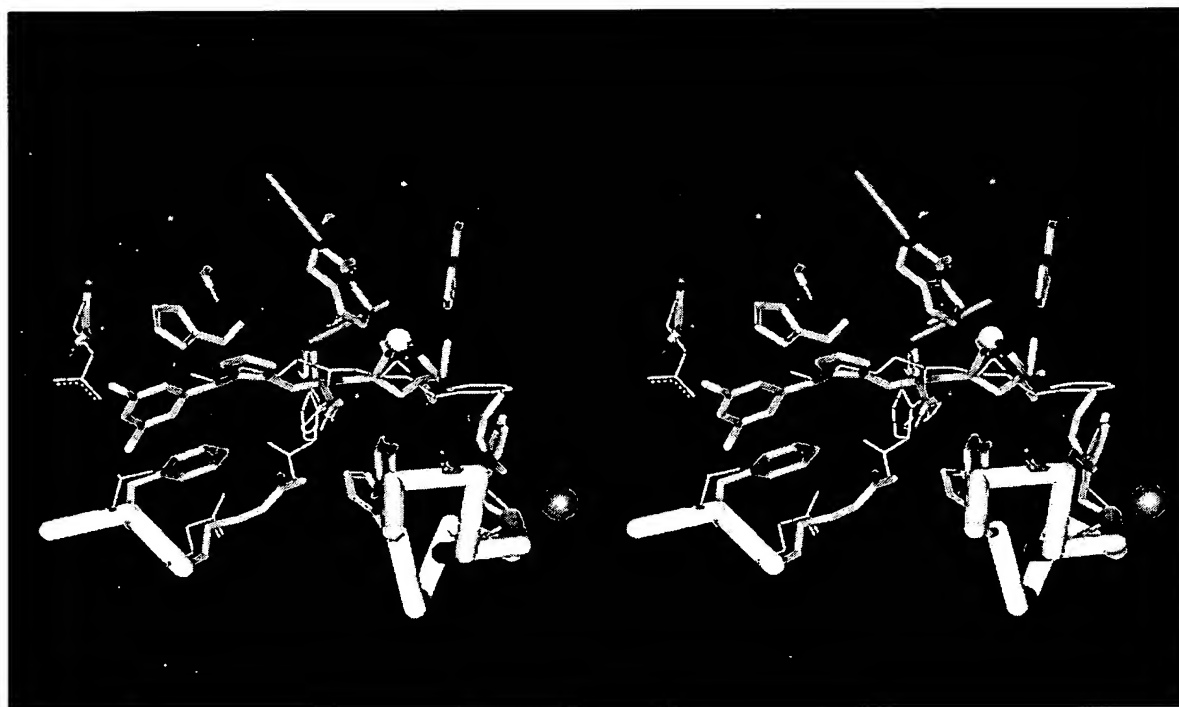


Figure 9B



392/396

Figure 10

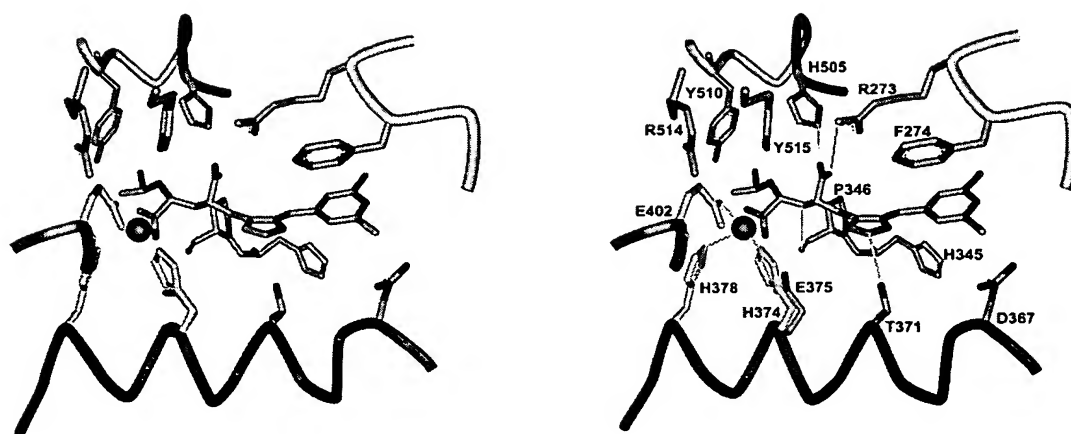


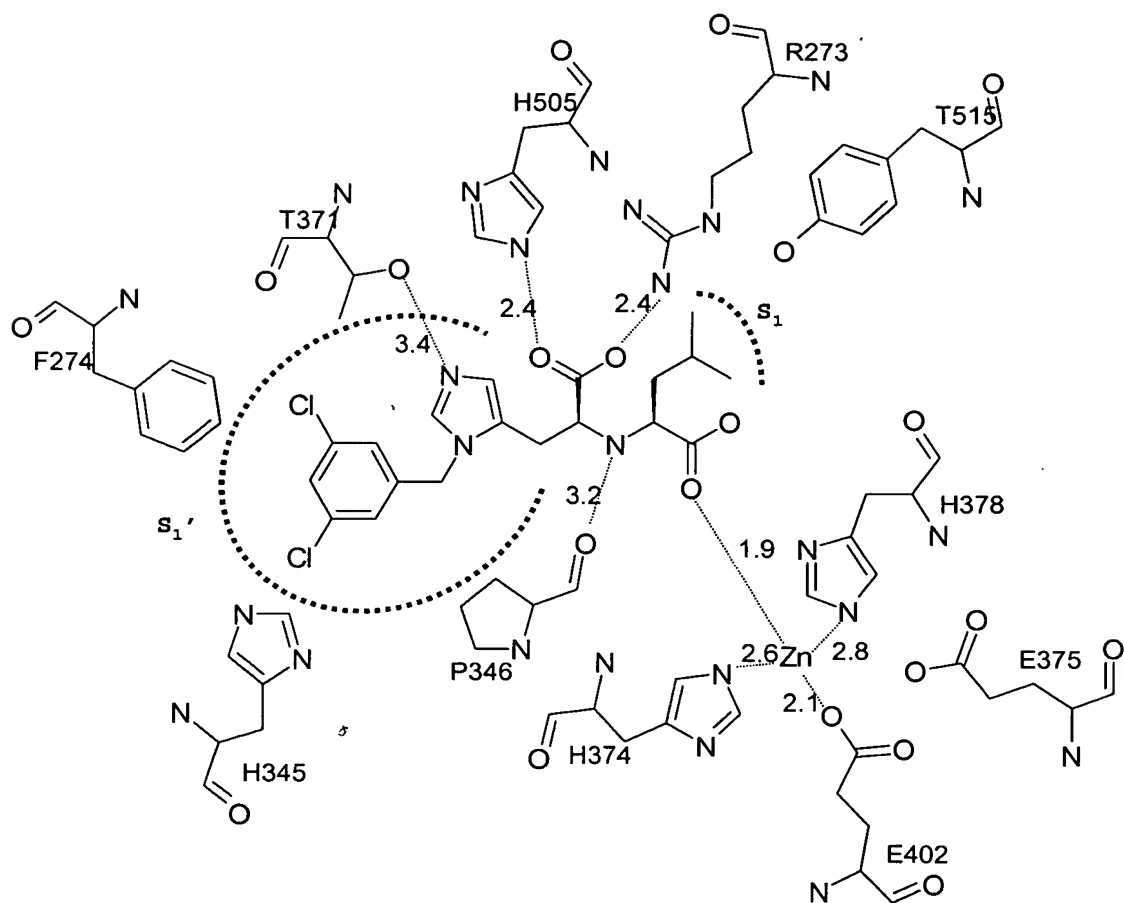
Figure 11

Figure 12

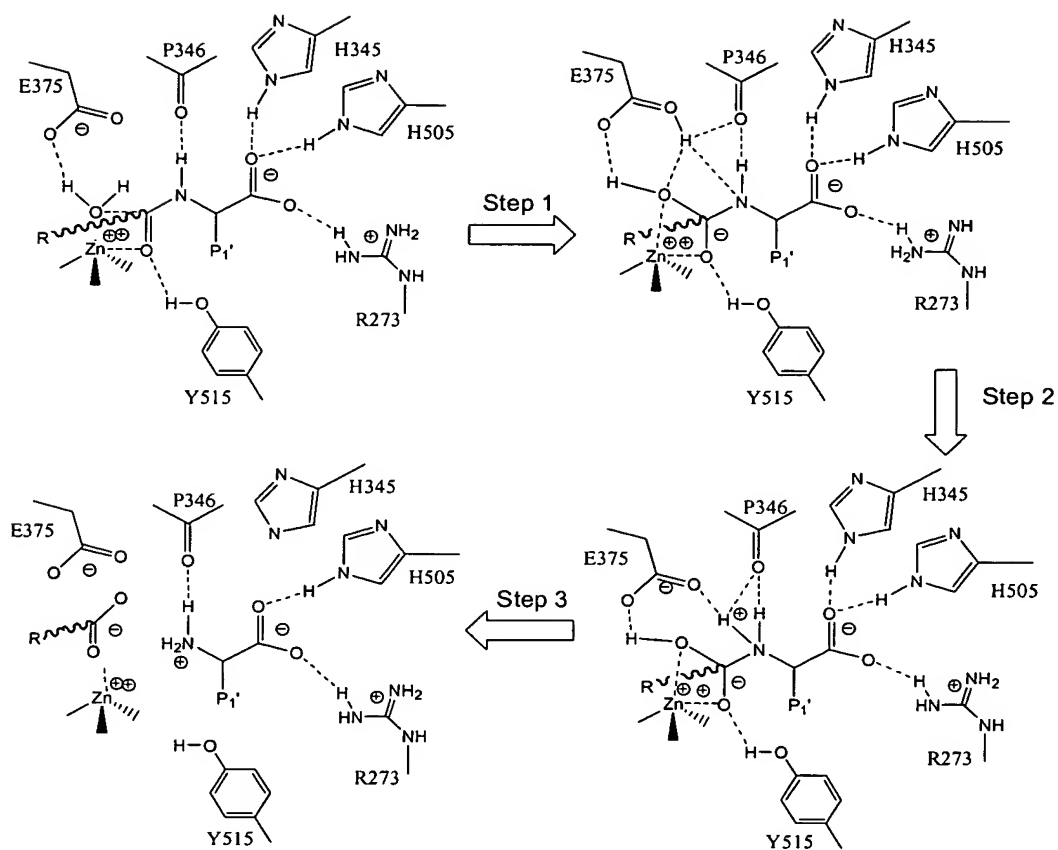


Figure 13

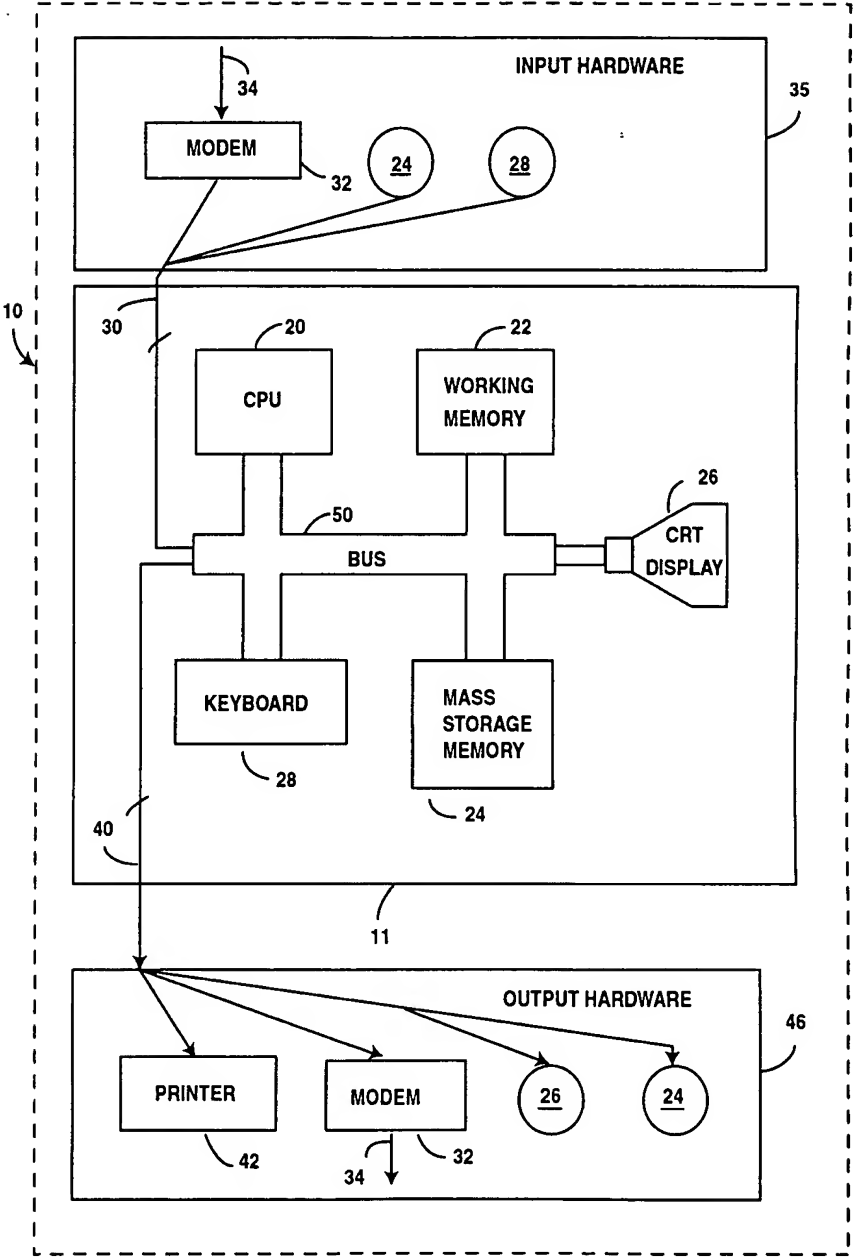


Figure 14

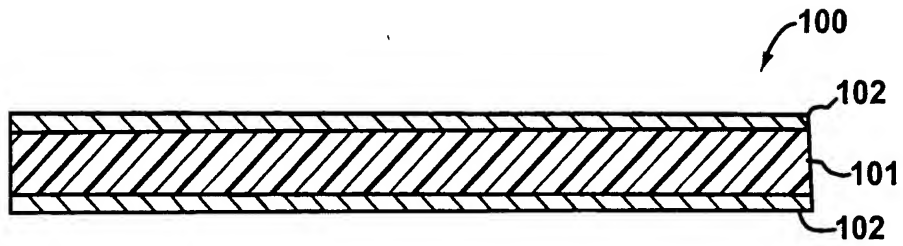


Figure 15

